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Solving Radial Component of Schrodinger Equation for Hydrogen Atom by wxmaxima

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Abstract— WxMaxima is a powerful tool for solving advanced mathematical operations. This can simplify mathematical equations and solve them, it can also plot the graphs, and compute derivatives and integration. For structural chemistry, atomic orbital calculation comprises a Laplacian Operator, associated polynomials, and functions of Laguerre. Using the example of the hydrogen atom, we propose a precise, quick, and feasible application method for solving the radial part of the H-atom equation, plot the graphs to illustrate the electronic cloud using wxMaxima

Indexed Terms-- Wxmaxima, Laplacian Operator, Laguerre polynomials

I. INTRODUCTION

We solve Schrödinger's equation for several instances. For example, the ground-state properties of electrons present in an atom, molecule, or solid can be described well using Schrodinger's equation. Therefore, it is necessary. to study hydrogen atom problems and observe precise electronic distribution, the shapes of orbitals, and their orientations [1]. Also, the solution of Schrodinger's equation in reciprocal space gives rise to electronic band structure and explains the origin of the bandgap with band theory which further executes the classification of solids into metals, semiconductors, and insulators [2]. The solution of Schrodinger's equation results in quantized properties of the quantum particles. Hence, in today's world, energy quantization is played a key role in fabricating quantum devices such as laser diodes and light-emitting diodes. Most of the semiconductor properties such as the behaviour of dopants and their energy levels present concerning the observed band structure etc are well explained after solving Schrodinger's equations [3].

Today it is possible to obtain the suitable dopants for a given semiconductor just by solving the corresponding Schrodinger's equation, before conducting the experiment on pure materials the real estimation of dopants and creating defects can be possible by solving the corresponding Schrodinger's equation. The ground-state properties of these defects can be well described [4]. Solving Schrodinger's equation for a solid involves the solution of complex differential equations [5]. The problem can be worked by expressing the differential Schrodinger's equation in momentum space in which the differential Schrodinger's equation is expressed as a set of linear algebraic equations rather than complex differential equations. Those linear equations can be solved using available computational numerical techniques accurately to predict the ground-state properties of solids [6]. Hence, performing calculations based on Schrodinger's equation using suitable computational methods makes the problem further simple and easy. It is possible to examine the physical system by interpreting the energies and wave functions of the system. Solving this equation by hand for a single-dimensional structure is an easy job, but when a three-dimensional case is considered, and the parameters are altered, it consumes more time and errors difficult to rectify. We use the wxMaxima to reach this challenge and quickly solve Schrodinger's equation. WxMaxima is easy and user-friendly to get a Schrodinger equation solution and to plot wave function results or probability densities etc. The commands used here are quick and easily writable. We can map 2d, and 3d plots by using wxMaxima and display two or more equations by simple commands in a single plot. We can also solve complicated functions and mathematical series, using certain commands and by calling the functions in the command

Hansen, J. has carried out their work on Mathematica for solving the time-independent Schrödinger equation [7]. Tellinghuisen et al dealt with numerical arrangements of the one-dimensional time-independent Schrödinger equation [8]. Ge, Y. et al performed their work by Utilizing a spreadsheet to solve the Schrödinger equations for the energies of the ground electronic state and the two lowest states of H_2.[9] However, wxMaxima is a tool that was not used to solve Schrodinger's equation. This paper intends to use wxMaxima to simplify complex mathematical calculations and to clarify the aspects of mathematics clearly and simply

II. METHOD

Hydrogen is the simplest element and the most common element in the universe. It consists of only a positively charged proton with a negatively charged orbiting electron. The proton has a mass much larger than the electron and is assumed to be located at the origin of the centre of mass of the system. It is assumed that the proton is stationary while the electron is orbiting it [10]. A system of the hydrogen atom is best described using spherical coordinates [11]. The electron is moving in a Coulomb potential V (r). if $\psi(r,\theta,\emptyset)$ is the probability density function of the electron, then the Schrodinger time-independent equation in spherical polar coordinates is given by

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

Considering the electron potential the above equation becomes,

$$-\frac{h^2}{8\pi^2 m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\,\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2 sin^2\theta}\frac{\partial}{\partial\phi^2}\right]\psi - \frac{Ze^2}{r}\psi = E\psi$$

The equation related to the above is a partial differential equation with variable (r, θ, ϕ) and the solution of this equation can be attempted by separating the variables and obtaining three specific differential equations [12]. Each of them will have a single variable.

$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\,\Phi(\phi)$

further simplification gives

$$\frac{sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{8\pi^2 mr^2 sin^2\theta}{h^2}\left(E+\frac{Ze^2}{r}\right)+\frac{sin\theta}{\Theta}\frac{d}{d\theta}\left(sin\theta\,\frac{d\Theta}{d\theta}\right)+\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=0 \qquad (1)$$

This equation is composed of each term with separate variables. Therefore, each equation can be solved separately

EQUATION OF RADIAL FUNCTION R(r)

Now equation (1) can be described for radial function as

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{8\pi^2 mr^2}{h^2}\left(E+\frac{Ze^2}{r}\right)=l(l+1)$$

and

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}\left[\frac{8\pi^2 mE}{h^2}+\frac{8\pi^2 mZe^2}{h^2 r}-\frac{l(l+1)}{r^2}\right]R=0$$

The above equation is 2^{nd} order differential equation and its solution is

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

In the case of a hydrogen atom, atomic number Z = 1 then

$$R_{n,l}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3\frac{(n-l-1)!}{2n[(n+1)!]^3}}\,e^{-\frac{r}{na_0}}\left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right) \quad (2)$$

Where, $L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)$ is Laguerre polynomial [13] of $n+l$ degree and $(2l+1)^{th}$ derivative of $\left(\frac{2r}{na_0}\right)$

Laguerre function value can be directly obtained using wxMaxima [14] by using a simple command diff (Laguerre(1,x),x,1); i.e. $L_1^1(x) = -1$

We will consider other Laguerre functions in the same way

For solving ordinary differential equation, we can use following commands

```
(%i1)    ode2('diff(Ψ,x,2)+2*m*Ψ*(E-V)/(ћ^2)=0,Ψ,x);
"Is "(V-E)*m" positive, negative or zero?"positive;
```

```
(%o1)	Ψ=%k1*%e^((%i*sqrt(2*E*m-2*V*m)*x)/ħ)+%k2*%e^(-(%i*sqrt(2*E*m-2*V*m)*x)/ħ
```

While for finding Laguerre polynomial [15], the commands used are

```
-->	laguerre(1,x);
(%o1)	1-x
-->	laguerre(2,x);
(%o2)	x^2/2-2*x+1
```

Result and discussion:

Graphs of radial wave function and radial probability density

For the ground state of the hydrogen atom, the quantum number of their possible values is appropriate.

For s-orbit n = 0,1, 2, 3 and l = 0.

For 1s orbit n = 1, l = 0 and a_0 = 0.529A^0= 0.529 ×10^{-10} m, $L_{1-0}^{2(o)+1}\left(\frac{2r}{na_0}\right) = L_1^0\left(\frac{2r}{na_0}\right) = -1$

$$R_{1,0}(r) = 2a_0^{-\frac{3}{2}}e^{-\frac{r}{a_0}} \qquad \ldots\ldots (3)$$

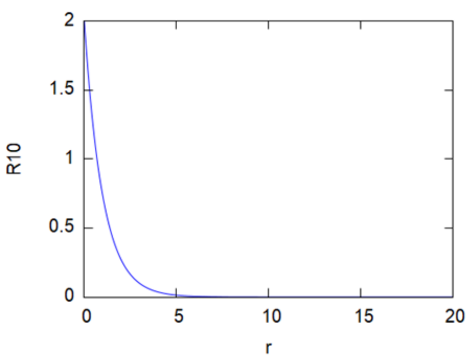


Fig (1): a plot of $\bar{R}_{1,0} = a_0^{-3/2}R_{1,0}$ verses $\left(\frac{r}{a_0}\right)$

Equation (3) plotted in above graph using wxMaxima [14,15,16] with commands shown

```
(%i1) load(implicit_plot)$
(%i2) R10(r) :=2*exp(-r) $
(%i3) wxplot2d ([R10],[r,0,20],[y,0,2]) $
```

Fig (1) shows the plot of the function **R$_{1,0}$(r)** against ***r***. It shows that the function goes maximum at r =0 and decays exponentially with r and there is no radial node

For 2s orbit n = 2, l = 0 and a_0 = 0.529A^0= 0.529 ×10^{-10} m,

$$L_{2-0}^{2(o)+1}\left(\frac{2r}{na_0}\right) = L_2^1\left(\frac{2r}{na_0}\right)$$
$$= 3\left(\frac{2r}{na_0}\right)^2 - 18\left(\frac{2r}{na_0}\right) + 18$$

$$R_{2,0}(r) = \frac{1}{\sqrt{2}}a_0^{-\frac{3}{2}}\left(1 - \frac{r}{2a_0}\right)e^{-\frac{r}{a_0}}$$
......(4)

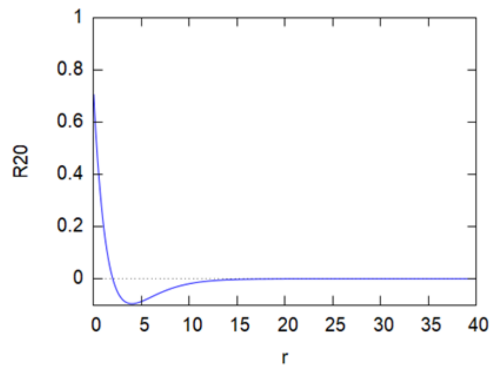


Fig (2) is a plot of $\bar{R}_{2,0} = a_0^{3/2}R_{2,0}$ verses $\left(\frac{r}{a_0}\right)$

Equation (4) plotted in above graph using wxMaxima with commands shown

```
(%i4)	R20(r) := (1/(sqrt(2)))*(1-r/2)*exp(-r/2) $
(%i5) wxplot2d ([R20],[r,0,40],[y,-0.1,1]) $
```

However, the radial wave function R$_{2,0}$(r) in fig (2) also decays exponentially, and further, it goes negative at $\frac{r}{a_0} \cong 2$, this point is called a radial node, it is a clear indication of the 2s orbit of the H atom

For 3s orbit n = 3, l = 0 and a_0 = 0.529A^0= 0.529 ×10^{-10} m,

$$L_{3-0}^{2(o)+1}\left(\frac{2r}{na_0}\right) = L_3^1\left(\frac{2r}{na_0}\right)$$
$$= -4\left(\frac{2r}{na_0}\right)^3 + 48\left(\frac{2r}{na_0}\right)^2 - 144\left(\frac{2r}{na_0}\right) + 96$$

$$R_{3,0}(r) = \frac{2}{\sqrt{27}}a_0^{-\frac{3}{2}}\left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2}\right)e^{-\frac{r}{3a_0}}$$
(5)

Equation (5) plotted in above graph using wxMaxima with commands shown

```
(%i6)	R30(r) :=(2/(sqrt(27)))*(1-(2*r/3)+(2*r^2/27))*exp(-r/3) $
```

(%i7)   wxplot2d ([R30],[r,0,25],[y,-0.1,0.4])$

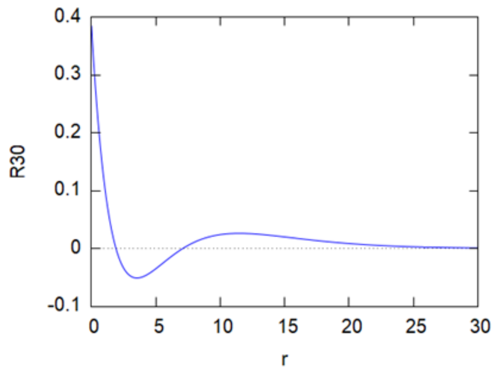


Fig (3) is a plot of $\bar{R}_{3,0} = a_0^{\frac{3}{2}} R_{3,0}$ verses $\left(\frac{r}{a_0}\right)$

Fig (3) shows that $R_{3,0}(r)$ for 3s orbit decreases exponentially with *r* and shows two radial nodes at $\frac{r}{a_0} \cong 2\ and\ \frac{r}{a_0} \cong 7$ [17]

Radial probability density: –

The function $R_{n,l}^2(r)r^2$ gives radial probability densities [17,18] for the hydrogen atom. The radial probability densities are plotted against r in the following figures

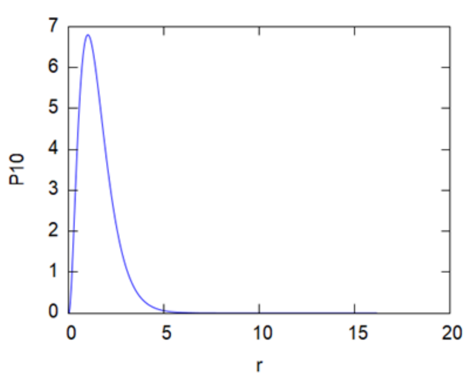


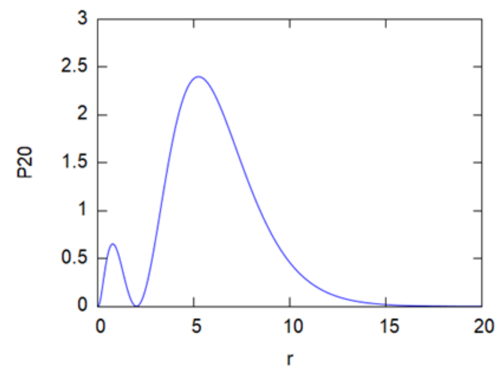
Fig (4): plot of the radial probability density function $R_{1,0}^2(r) 4\pi r^2 a_0$ verses $\left(\frac{r}{a_0}\right)$

wxMaxima Commands -

(%i8) P10(r) :=(16)*(π)*(r^2)*exp(-2*r) $

(%i9)wxplot2d(P10],[r,0,20],[y,0,7]) $

The probability density of radial wave function $4\pi r^2 R^2(r)$ for 1s orbit fig (4), shows a peak, which goes maximum at $\left(\frac{r}{a_0}\right) = 1$, therefore $r = a_0$. It is Bohr's 1st orbit with radius $a_0 = 0.529 \times 10^{-10}$ m



Fig(5) is a plot of a radial probability density function $R_{2,0}^2(r) 4\pi r^2 a_0$ verses $\left(\frac{r}{a_0}\right)$

wxMaxima Commands

(%i10) P20(r) :=(2)*(%pi)*(r^2)*(1-r/2)^2*(exp(-r)) $

(%i11) wxplot2d([P20],[r,0,20],[y,0,3]) $

Fig (5) the plot shows, for *2s* orbit shows two peaks, maxima at $\left(\frac{r}{a_0}\right) \cong 5$, therefore $r \cong 5a_0$, it is Bohr's 2nd orbit of radius $r = 4a_0$

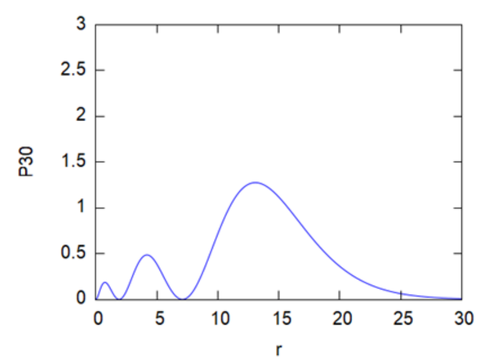


Fig (6) is the plot of a radial probability density function $R_{3,0}^2(r) 4\pi r^2 a_0$ verses $\left(\frac{r}{a_0}\right)$

wxMaxima Commands -

(%i12) P30(r) :=(16/27)*%pi*(r^2)*exp(-2*r/3)*(1-(2*r/3)+(2*r^2/27))^2 $

(%i13) wxplot2d([P30],[r,0,30],[y,0,3]) $

It shows for 3s orbit shows two peaks, maxima at $(r/a_0) \cong 13$, therefore $r \cong 13a_0$, is its Bohr's 3rd orbit of radius $r=9a_0$[18]

CONCLUSION

The radial wave function of a hydrogen atom depends on the principal quantum number and orbital quantum number. Graphs (1), (2), and (3) interpret each radial wave function of the H-atom obtained which can be used to determine the energy spectrum of the hydrogen atom, and radial probability graphs (4), (5), and (6) to find the electron at a distance 'r' from the centre of an atom.

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