Answer (a):-

Since, TISE is of the form:-

$$\nabla^2 \psi + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

Now, we have to determine the Laplace operator in spherical coordinate :-

$\because$ $x = r\sin\theta\cos\phi$

$y = r\sin\theta\cdot\sin\phi$

$z = r\cos\theta$

$\because$ $r^2 = x^2+y^2+z^2$

& $\tan\phi = y/x$

Thus Schrodinger equ^n in Polar coordinate is:-

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

This is schrodinger equ^h in spherical coordinate.

Since, S·E in polar form is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$

$$+\frac{2m}{\hbar^2}(\varepsilon-V)=0$$

Multiply by $r^2\sin\theta$:-

$$\sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{\partial^2\psi}{\partial\phi^2}$$

$$+\frac{2mr^2\sin^2\theta}{\hbar^2}(\varepsilon-V)\psi=0 \quad — (1)$$

$\because$ ψ is $\psi(r,\theta,\phi)=R(r)\cdot P(\theta)\cdot \Theta(\phi)$. — (2)

Putting (2) in (1) :-

$$\frac{1}{R(r)}\sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)+\frac{\sin\theta}{P(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{dP(\theta)}{d\theta}\right)$$

$$+\frac{1}{\Theta(\phi)}\frac{\partial^2\Theta\phi}{\partial\phi^2}+\frac{2mr^2\sin^2\theta}{\hbar^2}(\varepsilon-V)=0$$

2020PHY1216

Date : / /

$$\therefore \frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\sin\theta}{P}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right)+\frac{2mr^2\sin^2\theta}{\hbar^2}(\varepsilon-V)$$

$$=-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}$$

$\because$ L.H.S depends on r & θ & R.H.S to ϕ but they are equal to same constant :-

$$\therefore \frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\sin\theta}{P}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right)+\frac{2mr^2\sin^2\theta}{\hbar^2}(\varepsilon-V)=m^2$$

— (3)

dividing this by $\sin^2\theta$:-

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}(\varepsilon-V)=\frac{m^2}{\sin^2\theta}-\frac{1}{P\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right)$$

— (4)

Now, again equating to a constant :-

$$\left[\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}(\varepsilon-V)=l(l+1)\right]$$

— (5)

This is radial part.

2020 PHY1216

(b) :-

Now taking the radial part we get :-

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}(E-V)=l(l+1)$$

Since, $l=0$

$$\therefore \frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}(E-V)=0 \quad \text{— (*)}$$

Now, putting $R=\frac{K}{r}$

$$\therefore \frac{dR}{dr}=\frac{\frac{dK}{dr}\cdot r-K}{r^2} \quad \text{— (1)}$$

$$\text{\&} \quad \frac{d}{dr}\left(r^2\frac{dR}{dr}\right)=2r\frac{dR}{dr}+r^2\frac{d^2R}{dr^2}$$

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)=\frac{2dK}{dr}-\frac{2K}{r}+r^2\frac{d^2R}{dr^2} \quad \text{— (2)}$$

Differentiating (1) again w.r.t r :-

$$\left[\frac{d^2R}{dr^2}=\frac{1}{r}\frac{d^2K}{dr^2}-\frac{2}{r^2}\frac{dK}{dr}+\frac{2K}{r^2}\right] \quad \text{— (3)}$$

2020 PHY1246

Page No.
Date : / /

Put ③ in ② :-

$$\left[\frac{d}{dr}\left(r^2 \frac{dR}{dr} \right) = r \frac{d^2k}{dr^2} \right]$$

Put this in (*) :-

$$\frac{r^2}{k} \frac{d^2k}{dr^2} + \frac{2mr^2}{\hbar^2}(E - V) = 0$$

$$\text{or} \quad \frac{r^2}{k} \frac{d^2k}{dr^2} - \frac{2mr^2}{\hbar^2}(V - E) = 0$$

multiplying both sides by $-\frac{\hbar^2}{2mr^2}$

$$\therefore \left[-\frac{\hbar^2}{2m} \frac{d^2k}{dr^2} + Vk = Ek \right]$$

Now, making r dimensionless :-

$$\therefore r = \xi a_0$$

where, a_0 is Bohr radius

$$\therefore a_0 = \frac{k\hbar^2}{me^2}$$

then, $V(r) = \frac{-e^2}{kr} \cdot e^{-r/a}$

$$= \frac{-e^2}{k^2\hbar^2\xi} \cdot me^2 \cdot e^{-r/a}$$

2020 Phy1 2H

Also, $r^2 = \xi^2 a_0^2$

$$= \xi^2 \frac{k^2\hbar^4}{m^2e^4}$$

then $$\frac{\hbar^2}{2mr^2} = \frac{\hbar^2}{2m\xi^2} \times \frac{m^2e^4}{k^2\hbar^4}$$

$$= \frac{me^4}{2\xi^2k^2\hbar^2}$$

Putting this in above equation we get,

$$\frac{me^4}{2k^2\hbar^2} \frac{\partial^2 u(\xi)}{\partial\xi^2} + u(\xi)\frac{e^4}{k^2\hbar^2\xi} e^{-r/a} = E k$$

or $$\left[\frac{\partial^2}{\partial\xi^2} k(\xi) + 2k(\xi) \cdot \frac{e^{-r/a}}{\xi}\right] \frac{me^4}{2k^2\hbar^2} = -E k(\xi)$$

$$\Rightarrow \frac{\partial^2}{\partial\xi^2}[k(\xi)] + 2k(\xi) \cdot \frac{e^{-r/a}}{\xi} = e\, k(\xi)$$

here, $$\left[e = \frac{-E}{me^4} \times 2k^2\hbar^2\right]$$

where, e is dimensionless quantity with term $\frac{-me^4}{2k^2\hbar^2}$ being the ground state energy.

Page No.
Date : / /

2020PHY1216

$\therefore$ Equation becomes :-

$$\left[\frac{d^2}{d\xi^2} k(\xi) + \frac{2k}{\xi} \cdot e^{-\xi(q_0/a)} = e\, k(\xi) \right]$$

1 Discussion

1. Here I am plotting the Radial wavefunction for different value of ratio given in the assignment for *l=0*. We can conclude from the graph that as the ratio terms increases the decaying nature of the graph become more sharp.

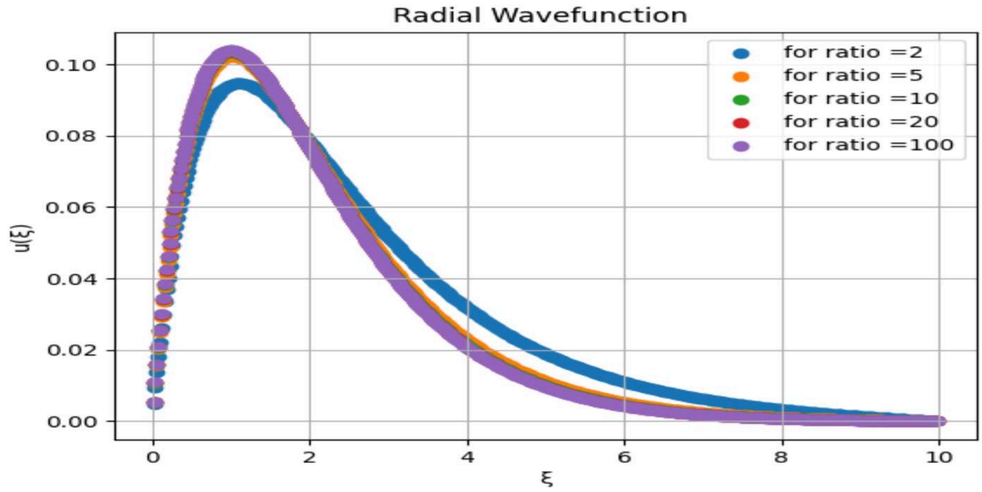

Figure 1:

2. This is the plot for the change in eigen values of the ground state with change in the ratio . We can clearly see that as the ratio increases the eigen value of the ground state approaches to the correct value i.e. 1

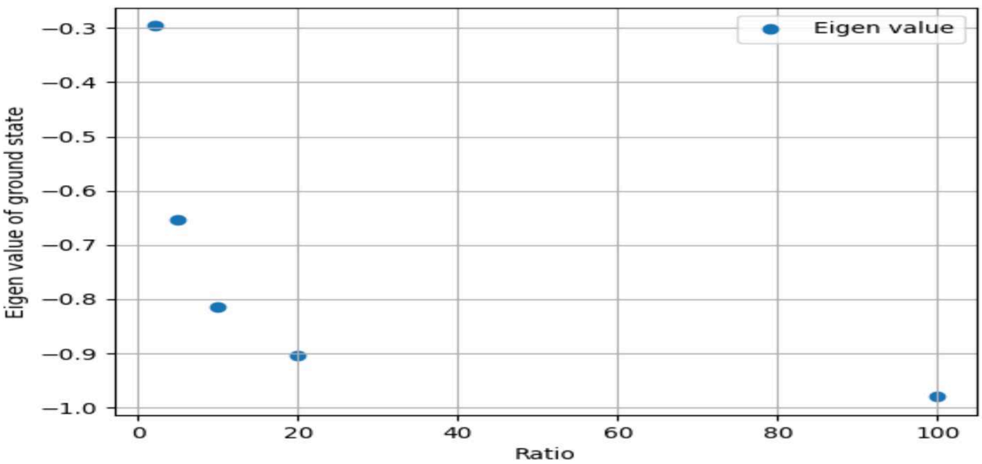

Figure 2:

3. This plot shows Probability Density of the waveform plotted above.

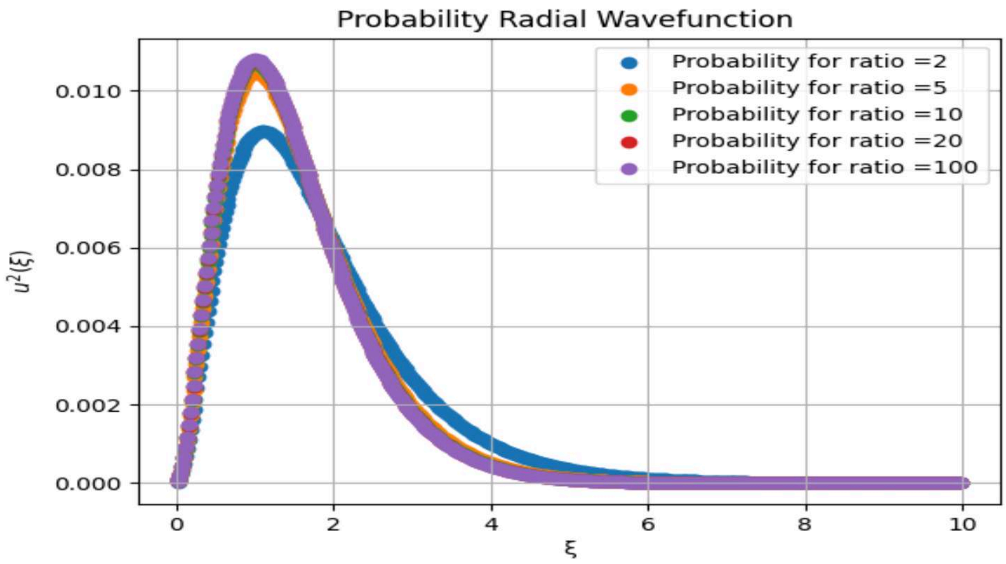

Figure 3:

4. Here I am plotting the Potential that we obtained in our case and the coulomb potential.

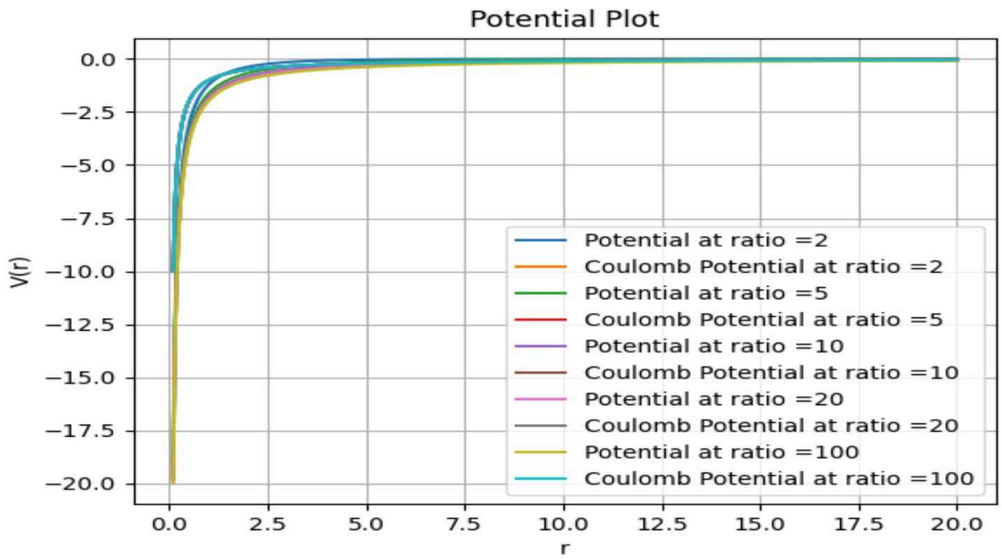

Figure 4:

5. This table have the values of the ground state eigen value with corresponding ratio.

```
[Running] python -u "d:\Download\5t
   Ratio  Eigen Value
0      2    -0.296063
1      5    -0.653516
2     10    -0.814015
3     20    -0.903532
4    100    -0.980048
```

Figure 5:

B.Sc.(Hons.) Physics	**S.G.T.B. Khalsa College**	Due Date and Time :
32221501	**Quantum Mechanics (2022-23)**	16.10.2022, 11:59PM
Teacher: Mamta	**Lab Assignment # 12**	Max. Marks : 20
	Screened Coulamb Potential	

This assignment is based on the Problem 2 of the syllabus.

1. (6 marks) **Theory**

   (a) The electron in an atom is subjected to the screened Coulomb Potential given by

   $$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}e^{-r/a} = V_c e^{-r/a}$$

   V_c being the Coulomb potential.

   Write down the Schrödinger Equation in spherical polar coordinates. Use separation of variables to obtain the radial part of the Schrödinger Equation for a given value of ℓ.

   (b) Now consider the radial equation for $\ell = 0$ and convert it into dimensionless form by redefining $r = \xi a_0$, a_0 being the Bohr radius.

   (c) Plot the Coulamb potential V_c (in dimensionless form) and on the same graph, plot the potential $V(\xi) = V_c e^{-\xi/\alpha}$ as a function of ξ for different values of $\alpha = \frac{a}{a_0}$, say $\alpha = 2, 5, 10, 20, 100$. Discuss what do you expect for the bound state eigen values.

2. (12 marks) **Programming** Write a Python code to solve the s-wave ($\ell = 0$) Schrödinger Equation for an atom (in dimensionless form) for the screened Coulamb Potential

   $$V(\xi) = V_{\text{coul}} e^{-\xi/\alpha}$$

   The code should

   (a) obtain the bound state energy eigen values. Is the number of bound state finite?

   (b) obtain the the energy (in eV) of the ground state of the atom to an accuracy of three significant digits for the values of α mentioned above. Take $e = 3.795(eV\AA)^{1/2}$, $m = 0.511$ MeV/c^2. In these units $\hbar c = 1973(eV\AA)$.

   (c) plot the corresponding normalised wavefunctions. Also plot the wavefunctions for the Coulamb potential on the same graph.

   (d) plot the probability densities

   (e) plot the ground state energy as a function of α

3. (2 marks) **Discussion**

   Read the article shared with you. Interpret and discuss your results.