Assignment 12 - Screened Coulomb Potential

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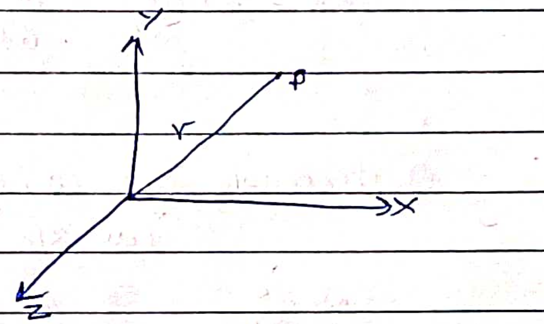
Theory

(a) Write Schrodinger Equation for an electron in H-atom potential in spherical coordinates.

Ans: The potential energy of a particle moving under central spherically symmetric field of force has the form $V(r)$ where r is distance b/w particle and centre of force. The schrodinger eqn for such system

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

$$\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\psi + \frac{2m}{\hbar^2}[E-V(r)]\psi = 0 \quad -(1)$$

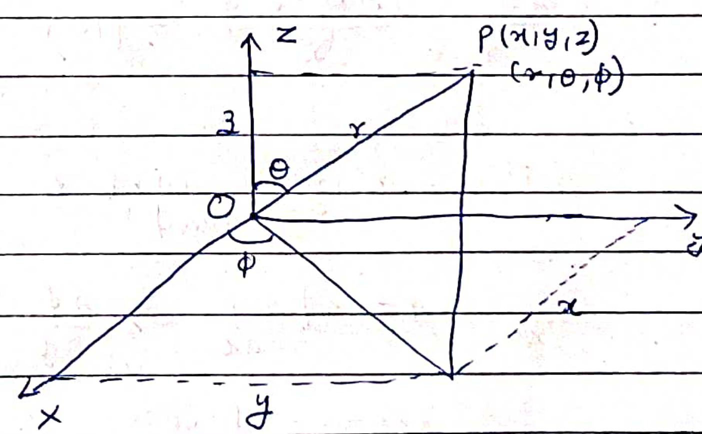


The relation between spherical & cartesian coordinate system is:

$x = r\sin\theta\cos\phi \quad -(2)$

$y = r\sin\theta\sin\phi \quad -(3)$

$z = r\cos\theta \quad -(4)$



(3)/(4) gives

$\frac{y}{x} = \tan\phi \quad -(5)$

From (4) $\cos\theta = z/r \quad -(6)$

square (2) (3) (4) & add

$$x^2+y^2+z^2 = r^2\sin^2\theta\cos^2\phi + r^2\sin^2\theta\sin^2\phi + r^2\cos^2\theta$$

$$= r^2\sin^2\theta(\cos^2\phi+\sin^2\phi) + r^2\cos^2\theta$$

$$\boxed{x^2+y^2+z^2 = r^2} \quad -(7)$$

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Let's take ψ in terms of polar coordinates $(r, \theta, \phi) \Rightarrow \psi(r, \theta, \phi)$

$$\psi = \psi(r, \theta, \phi)$$

$$\frac{d\psi}{dx} = \frac{\partial \psi}{\partial r} \times \frac{\partial r}{\partial x} + \frac{\partial \psi}{\partial \theta} \times \frac{\partial \theta}{\partial x} + \frac{\partial \psi}{\partial \phi} \times \frac{\partial \phi}{\partial x} \quad (8)$$

Differentiate (7) w.r.t x

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

$$\cancel{2}x = \cancel{2}r \frac{dr}{dx} \quad \frac{dr}{dx} = \frac{x}{r} = \frac{\cancel{r} \sin\theta \cos\phi}{\cancel{r}} = \sin\theta \cos\phi \quad -(9)$$

Differentiate (6) w.r.t. x

$\cos\theta = z/r$

$$-\sin\theta \frac{\partial \theta}{\partial x} = \frac{-z}{r^2} \frac{\partial r}{\partial x} \Rightarrow \frac{-z}{r^2} \times \sin\theta \cos\phi = \frac{-r \cos\theta \cancel{\sin\theta} \cos\phi}{r^2}$$

$$\frac{\partial \theta}{\partial x} = \frac{\cos\theta \cos\phi}{r} \quad -(10)$$

Differentiate (5) w.r.t. x

$y/x = \tan\phi$

$$\frac{-y}{x^2} = +\sec^2\phi \frac{\partial \phi}{\partial x} \Rightarrow \frac{\partial \phi}{\partial x} = \frac{-y}{\sec^2\phi \times x^2} = \frac{-y \cos^2\phi}{x^2}$$

$$= \frac{-\cancel{r}\cancel{\sin\theta} \sin\phi \cancel{\cos^2\phi}}{r^{\cancel{2}} \sin^{\cancel{2}}\theta \cancel{\cos^2\phi}}$$

$$\frac{\partial \phi}{\partial x} = -\frac{\sin\phi}{r\sin\theta} \quad -(11)$$

Put (9), (10), (11) in (8)

$$\frac{\partial \psi}{\partial x} = \frac{\partial \psi}{\partial r} \times \sin\theta\cos\phi + \frac{\partial \psi}{\partial \theta} \times \frac{\cos\theta \cos\phi}{r} + \frac{\partial \psi}{\partial \phi} \frac{\sin\phi}{r \sin\theta} \quad (12)$$

As we know we need $\frac{\partial^2 \psi}{\partial x^2}$ in STISE

$$\frac{\partial}{\partial x} = \sin\theta\cos\phi \frac{\partial}{\partial r} + \cos\theta\cos\phi \frac{\partial}{\partial \theta} - \frac{\sin\phi}{r\sin\theta} \frac{\partial}{\partial \phi} \quad (13)$$

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$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial \psi}{\partial x}\right)$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial}{\partial x}\frac{\partial \psi}{\partial r}\times\frac{\partial r}{\partial x} + \frac{\partial}{\partial x}\frac{\partial \psi}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial}{\partial x}\frac{\partial \psi}{\partial \phi}\frac{\partial \phi}{\partial x}$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial}{\partial r}\frac{\partial \psi}{\partial x}\frac{\partial r}{\partial x} + \frac{\partial}{\partial \theta}\frac{\partial \psi}{\partial x}\frac{\partial \theta}{\partial x} + \frac{\partial}{\partial \phi}\frac{\partial \psi}{\partial x}\frac{\partial \phi}{\partial x} \quad - (14)$$

Putting 9, 10, 11, 12 in (14) gives

$$\frac{d^2 \psi}{\partial x^2} = \frac{\partial}{\partial r}\left[\sin\theta\cos\phi\frac{\partial \psi}{\partial r} + \frac{\cos\theta\cos\phi}{r}\frac{\partial \psi}{\partial \theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial \psi}{\partial \phi}\right]\sin\theta\cos\phi$$

$$+\frac{\partial}{\partial \theta}\left[\ ---\ \right]\frac{\cos\theta\cos\phi}{r} + \frac{\partial}{\partial \phi}\left[\ ----\ \right]\frac{-\sin\phi}{r\sin\theta} \quad - (15)$$

Similarly $\frac{\partial^2 \psi}{\partial y^2}$ will come out to be

$$\frac{\partial \psi}{\partial y} = \sin\theta\sin\phi\frac{\partial \psi}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial \psi}{\partial \theta} + \frac{\cos\phi}{r\,\cancel{\cos}\sin\theta}\frac{\partial \psi}{\partial \phi} \quad (19)$$

$$\frac{\partial r}{\partial y} = \sin\theta\sin\phi \quad -(16)$$

$$\frac{\partial \theta}{\partial y} = \frac{\cos\theta\sin\phi}{r} \quad -(17)$$

$$\frac{\partial \phi}{\partial y} = \frac{\cos\phi}{r\,\cancel{\cos}\sin\theta} \quad -(18)$$

$$\frac{\partial^2 \psi}{\partial y^2} = \frac{\partial}{\partial r}\left(\frac{\partial \psi}{\partial y}\right)\left(\frac{\partial r}{\partial y}\right) + \frac{\partial}{\partial \theta}\left(\frac{\partial \psi}{\partial y}\right)\left(\frac{\partial \theta}{\partial y}\right) + \frac{\partial}{\partial \phi}\left(\frac{\partial \psi}{\partial y}\right)\left(\frac{\partial \phi}{\partial y}\right) - (20)$$

Put 16, 17, 18, 19 in (20

$$\frac{\partial^2 \psi}{\partial y^2} = \frac{\partial}{\partial r}\left[\sin\theta\sin\phi\frac{\partial \psi}{\partial r} + \frac{\cos\theta\sin\phi}{r}\frac{\partial \psi}{\partial \theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial \psi}{\partial \phi}\right]\sin\theta\sin\phi +$$

$$\frac{\partial}{\partial \theta}\left[\ ---\ \right]\frac{\cos\theta\sin\phi}{r} + \frac{\partial}{\partial \phi}\left[\ ---\ \right]\frac{\cos\theta}{r\sin\theta} \quad -(21)$$

To find $\frac{\partial^2\psi}{\partial z^2}$, we've $\frac{\partial\psi}{\partial z} = \frac{\partial\psi}{\partial r}\frac{\partial r}{\partial z} + \frac{\partial\psi}{\partial\theta}\frac{\partial\theta}{\partial z} + \frac{\partial\psi}{\partial\phi}\frac{\partial\phi}{\partial z}$ -(25)

$\frac{\partial r}{\partial z} = \cos\theta$ -(22) $\quad \frac{\partial\theta}{\partial z} = -\frac{\sin\theta}{r}$ -(23) $\quad \frac{\partial\phi}{\partial z} = 0$ -(24)

Putting (22), (23), (24) in (25)

$$\frac{\partial\psi}{\partial z} = \cos\theta\frac{\partial\psi}{\partial r} - \frac{\sin\theta}{r}\frac{\partial\psi}{\partial\theta} \quad -(26)$$

Now,
$$\frac{\partial^2\psi}{\partial z^2} = \frac{\partial}{\partial r}\left(\frac{\partial\psi}{\partial z}\right)\left(\frac{\partial r}{\partial z}\right) + \frac{\partial}{\partial\theta}\left(\frac{\partial\psi}{\partial z}\right)\left(\frac{\partial\theta}{\partial z}\right) + \frac{\partial}{\partial\phi}\left(\frac{\partial\phi}{\partial z}\right)\left(\frac{\partial\phi}{\partial z}\right) \quad -(27)$$

Putting 22, 23, 24, 26 in 27

$$\frac{\partial^2\psi}{\partial z^2} = \frac{\partial}{\partial r}\left[\cos\theta\frac{\partial\psi}{\partial r} - \frac{\sin\theta}{r}\frac{\partial\psi}{\partial\theta}\right]\cos\theta + \frac{\partial}{\partial\theta}\left[\cos\theta\frac{\partial\psi}{\partial r} - \frac{\sin\theta}{r}\frac{\partial\psi}{\partial\theta}\right]\left[\frac{-\sin\theta}{r}\right] \quad -(28)$$

Add (15), (21) & (28)

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} \quad (29)$$

Using (29) in

$$\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + \frac{2m}{\hbar^2}\left[E - V(r)\right]\psi \text{ is}$$

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

(b) Use separation of variable method to separate this into angular & radial part. (Use $\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_{\ell m}(\theta,\phi)$ & take separation constant $\ell(\ell+1)$.

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S.E in polar form is given as:-

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

Multiply both sides by $r^2\sin^2\theta$

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

Take $\psi(r,\theta,\phi)=R(r)P(\theta)Q(\phi) \quad -(2)$

Put (2) in (1)

$$\frac{1}{R(r)}\sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)+\frac{1}{P(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P(\theta)}{\partial\theta}\right)\sin\theta+\frac{1}{Q(\phi)}\frac{\partial^2 Q(\phi)}{\partial\phi^2}$$
$$+\frac{2m}{\hbar^2}(E-V)r^2\sin^2\theta=0$$

$$\frac{1}{R(r)}\sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)+\frac{1}{P(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P(\theta)}{\partial\theta}\right)\sin\theta+\frac{2m(E-V)r^2\sin^2\theta}{\hbar^2}$$
$$=-\frac{1}{Q(\phi)}\frac{\partial^2 Q(\phi)}{\partial\phi^2}$$

L.H.S. depends on r and θ whereas RHS depends on φ, but LHS = RHS, so they can be equated to a constant m^2

$$\frac{1}{R(r)}\sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)+\frac{1}{P(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P(\theta)}{\partial\theta}\right)\sin\theta+\frac{2m(E-V)r^2\sin^2\theta}{\hbar^2}=m^2 \quad (3)$$

$$\frac{1}{R(r)}\cancel{\sin^2\theta}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)+\frac{1}{P(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P(\theta)}{\partial\theta}\right)\frac{1}{\sin\theta}+\frac{2m(E-V)r^2}{\hbar^2}=\frac{m^2}{\sin^2\theta}$$

Now again by separation of constant

$$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)-\frac{2m(E-V)r^2}{\hbar^2}=\frac{m^2}{\sin^2\theta}-\frac{1}{P(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P(\theta)}{\partial\theta}\right)\frac{1}{\sin\theta} \quad (4)$$

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Equate (4) with a constant

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

Radial Part

$$\frac{m^2}{\sin^2\theta} - \frac{1}{P(\theta)} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial P(\theta)}{\partial \theta}\right) \frac{1}{\sin\theta} = \ell(\ell+1)$$

Angular Part

For $v(r) = \frac{-e^2}{4\pi\varepsilon_0 r} e^{-r/a} = V_c e^{r/a}$

$V_{eff} = V_c e^{-r/a} + \frac{l(l+1)\hbar^2}{2mr^2}$

Take $l=0$, $r = \xi a_0$, $k = 4\pi\varepsilon_0$

$V_{eff} = V_c e^{-\frac{\xi a_0}{a}}$

here a_0 is bohr radius, $a_0 = \frac{k\hbar^2}{me^2}$

$v(r) = \frac{-e^2}{kr} e^{-r/a} = \frac{-e^2}{k^2\hbar^2\xi} me^2 e^{-r/a}$

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

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

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

The above eqn becomes,

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

$\frac{\partial^2}{\partial\xi^2}(k(\xi)) + 2k(\xi)\frac{e^{-r/a}}{\xi} = ek(\xi)$

here e is $-\frac{E\, 2k^2\hbar^2}{me^4}$

e is dimensionless & $-\frac{me^4}{2k^2\hbar^2}$ is ground state energy

The Eqn in dimensionless form is

$\frac{d^2}{d\xi^2} k(\xi) + \frac{2k}{\xi} e^{-\xi(a_0/a)} = ek(\xi)$

Programming

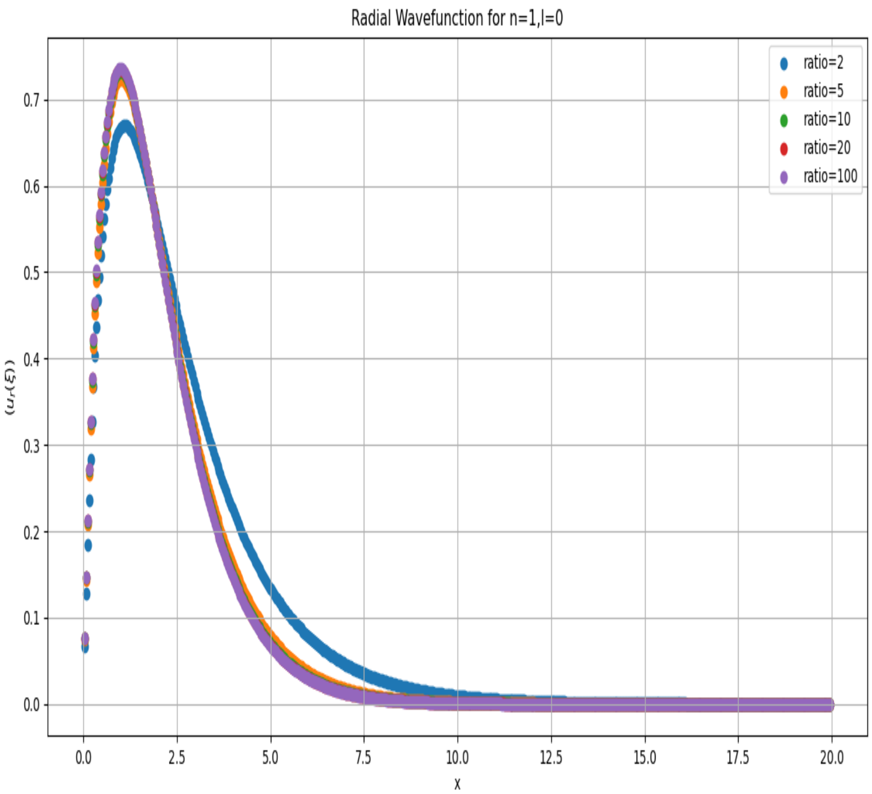
```python
import numpy as np
from scipy.linalg import eigh
import matplotlib.pyplot as plt
import scipy.integrate as integrate
import pandas as pd
from scipy.special import assoc_laguerre
from scipy.optimize import fsolve
def diag_mat(xi,xf,N,l,ratio):
    X = np.linspace(xi,xf,N+2)
    x=X[1:-1]
    h = x[1]-x[0]
    a,v=np.zeros((len(x),len(x))),np.zeros((len(x),len(x)))
    for i in range(len(x)):
        for j in range(len(x)):
            if i==j:
                a[i][i]=2/h**2
                v[i][i]=(-2/x[i])*np.exp(np.divide(-x[i],ratio))+((l)*(l+1))/(2*(x[i]**2))
            elif i==j+1:
                a[i][j]=-1/h**2
            elif i == j-1:
                a[i][j] = -1/h**2
    A=(a+v)
    eig = eigh(A)
    return eig,x
def V(x,ratio):
    v_x=(-2/x)*np.exp(np.divide(-x,ratio))
    v_coulomb = (-2/x)
    return v_x, v_coulomb
def graph(x,y,label,xlabel,ylabel,title):
    plt.scatter(x,y,label=f'ratio={j}')
    plt.xlabel(xlabel)
    plt.ylabel(ylabel)
    plt.title(title)
    plt.grid()
    plt.legend()

N=500
for i in range(0,1,1):
    xi=0;xf=20
    U_a=[];ratio_=[];v_x=[];v_coulomb=[]
    ratio_=[2,5,10,20,100]
    for j in ratio_:
        ratio=j
        U_,x=diag_mat(xi,xf,N,0,j)
        U=U_[1][:,i]
        U_a.append(U_[0][:1][0])
        u_norm=U/np.sqrt(integrate.simps(np.power(U,2),x))
        v_x, v_coulomb=V(x,j)
        # graph(x,v_x,j,"$\u03BE$","$V(\u03BE)$","Screened Coulomb Potential")
        # graph(x,v_coulomb,j,"$\u03BE$","$V_c$","Coulomb Potential")
        # graph(x,np.power(u_norm,1),j,"x","$(u_r(\u03BE))$","Radial Wavefunction for n=1,l=0")
        graph(x,np.power(u_norm,2),j,"x","$(u_r(\u03BE))^2$","Radial Probability for n=1,l=0")
plt.show()

#---------------------Q-a(ii)--------------------------#
p=[]
for i in range(1,len(ratio_)+1):
    p.append(-1/1**2)
data ={
    "ratio":ratio_,
    "Numerical Eigen Values ": U_a,
    # "Analytical Eigen Values ":p ,
```

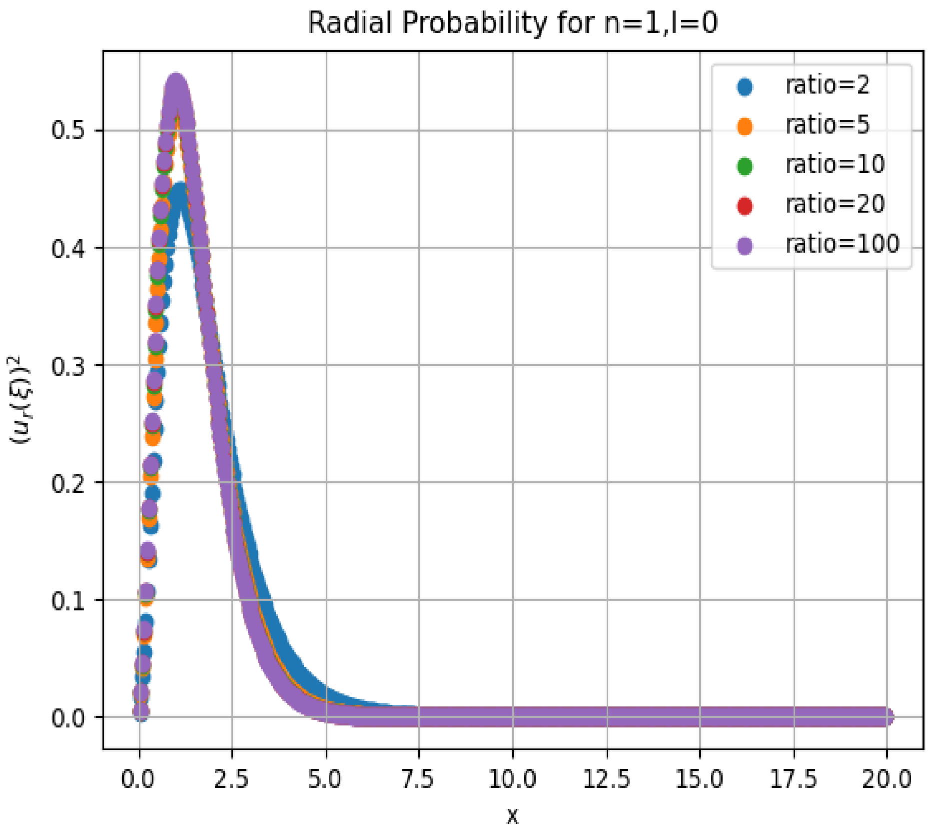
```
}
print(pd.DataFrame(data))
# plt.scatter(ratio_,U_a)
# plt.grid()
# plt.xlabel("ratio")
# plt.ylabel("Eigen Value")
# plt.show()
```

Result and Discussion

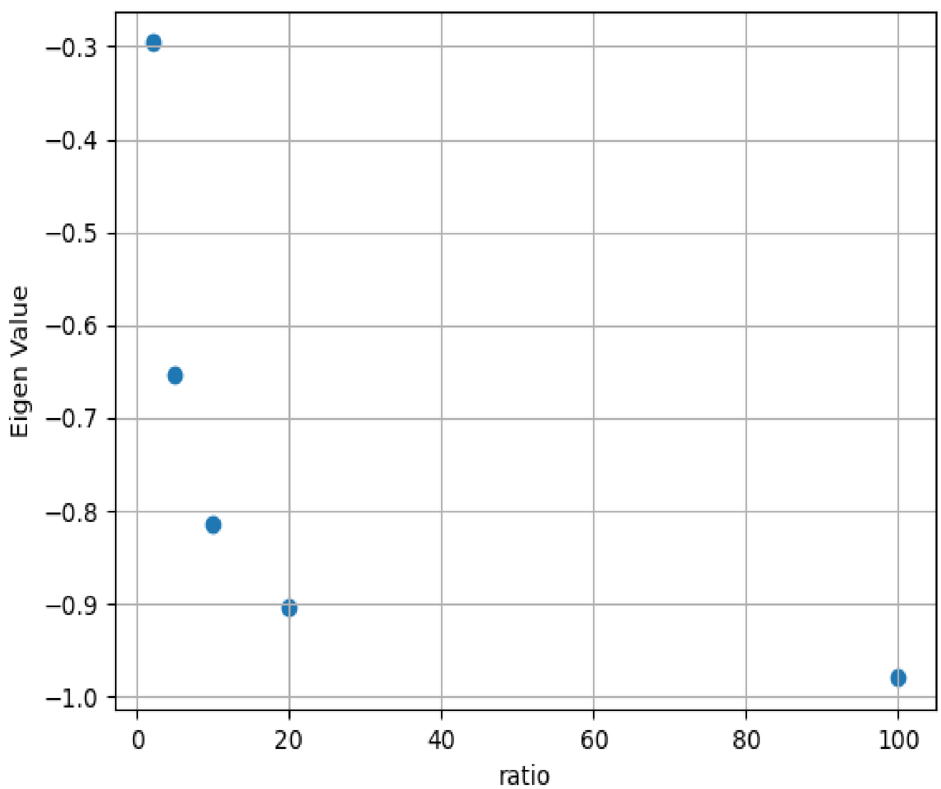
Bound Energy State Eigen Value for n=0

	ratio	Numerical Eigen Values
0	2	-0.295909
1	5	-0.653232
2	10	-0.813722
3	20	-0.903236
4	100	-0.979751

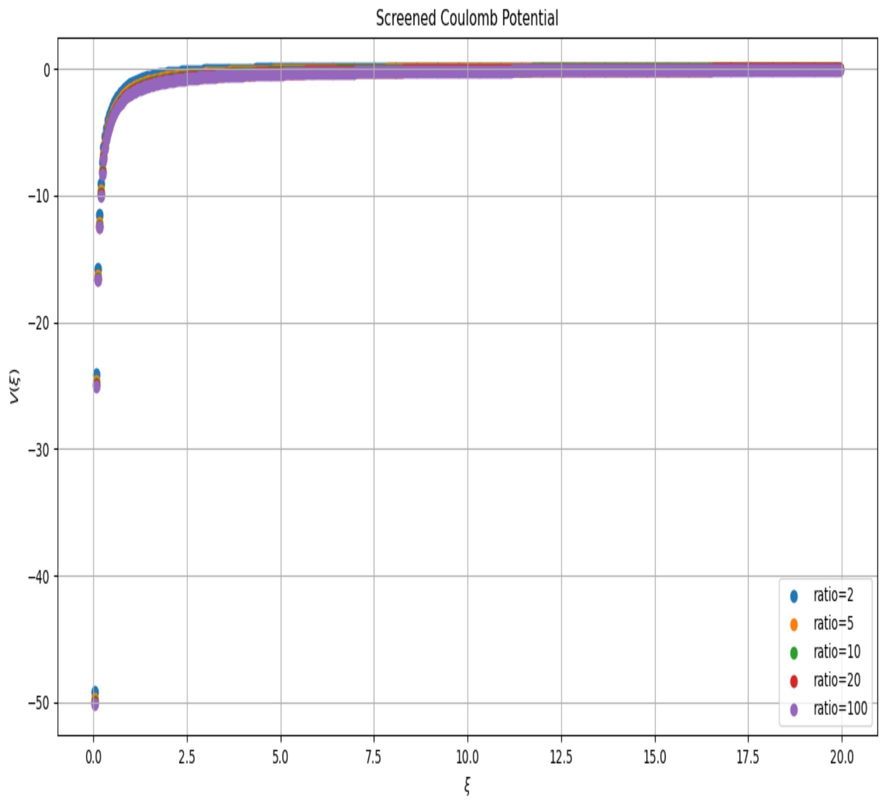

Radial Wavefunction for n=1,l=0
ratio=2
ratio=5
ratio=10
ratio=20
ratio=100
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
x

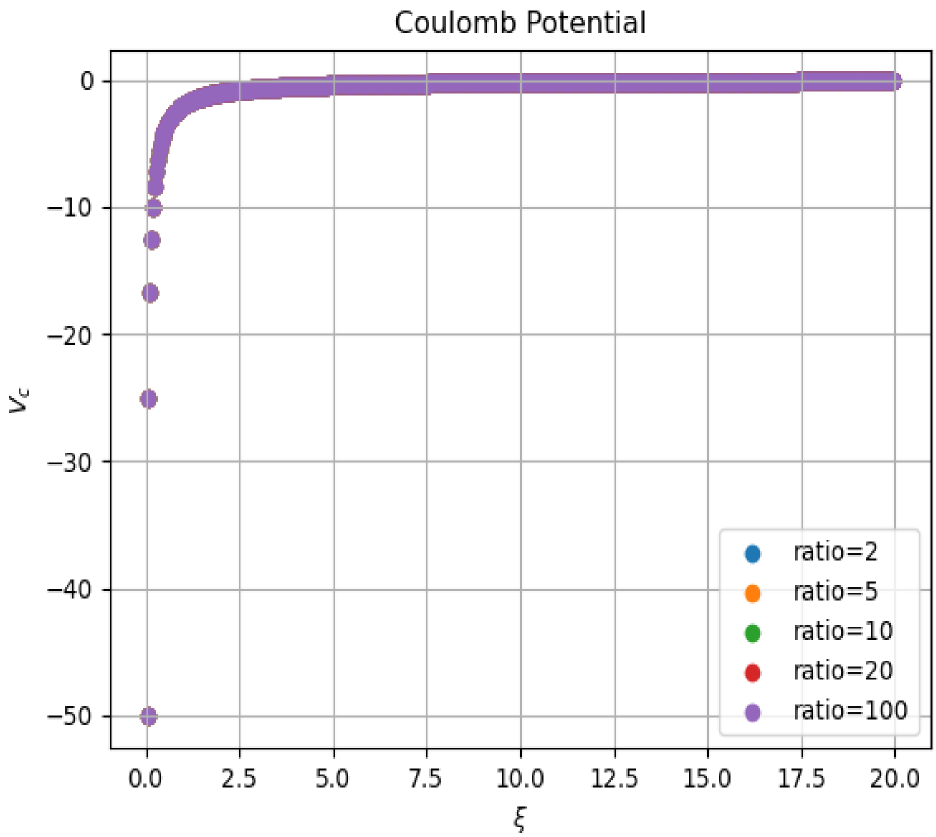


Radial Probability for n=1,l=0
ratio=2
ratio=5
ratio=10
ratio=20
ratio=100
$(u_r(\xi))^2$
x
0.0
0.1
0.2
0.3
0.4
0.5
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0



−0.3
−0.4
−0.5
−0.6
−0.7
−0.8
−0.9
−1.0
Eigen Value
0
20
40
60
80
100
ratio


Screened Coulomb Potential
0
−10
−20
−30
−40
−50
$V(\xi)$
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
ξ
ratio=2
ratio=5
ratio=10
ratio=20
ratio=100


Coulomb Potential
0
−10
−20
−30
−40
−50
v_c
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
ξ
ratio=2
ratio=5
ratio=10
ratio=20
ratio=100