Assignment 12 - Screened Coulomb Potential

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Theory :

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

TISE,

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

$$\psi(\vec{r}) = \psi(r, \theta, \phi)$$

we know,

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

$$+ \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$

$$\Rightarrow \frac{-\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \left(\frac{-\hbar^2}{2m}\right)\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)$$

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

$$= E\psi(r,\theta,\phi) \quad (1)$$

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\, Y_{lm}(\theta,\phi)$$

Substitute in (1)

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$$\Rightarrow \frac{-\hbar^2}{2m}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}(R_{nl}Y_{lm})\right) + \left(\frac{-\hbar^2}{2mr^2}\right)$$

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}R_{nl}Y_{lm}\right) + \frac{1}{\sin\theta}\frac{\partial^2}{\partial\phi^2}R_{nl}Y_{lm}\right]$$

$$+ V(r)R_{nl}Y_{lm} = E\,R_{nl}Y_{lm}$$

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

$$\Rightarrow \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}(R_{nl}Y_{lm})\right) + \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}(R_{nl}Y_{lm})\right)\right.$$

$$\left.+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}(R_{nl}Y_{lm})\right] - \frac{2mr^2}{\hbar^2}V(r)R_{nl}Y_{lm}$$

$$= -\frac{2mr^2}{\hbar^2}E(R_{nl}Y_{lm})$$

$R_{nl}(r)$ will only get diff. by $\frac{\partial}{\partial r}$

Y_{lm} will get diff by $\frac{\partial}{\partial\theta}$ and $\frac{\partial}{\partial\phi}$

$$\Rightarrow Y_{lm}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}(R_{nl})\right)\right] + R_{nl}\left[\frac{1}{\sin\theta}\left(\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}Y_{lm}\right)\right)\right.$$

$$\left.+\frac{1}{\sin\theta}\frac{\partial^2}{\partial\phi^2}(Y_{lm})\right) + \frac{2mr^2}{\hbar^2}(E-V(r))\,Y_{lm}R_{nl} = 0$$

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Dividing by $\psi_{n\ell m}(r,\theta,\phi) = Y_{\ell m}(\theta,\phi) R_{n\ell}(r)$

$$\Rightarrow \frac{1}{R_{n\ell}} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}(R_{n\ell})\right) + \frac{2mr^2}{\hbar^2}(E - V(r)) +$$

$$\frac{1}{Y_{\ell m}}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}(Y_{\ell m})\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}(Y_{\ell m})\right] = 0$$

Seperating angolar and radial part,

$$\Rightarrow \frac{1}{R_{n\ell}} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}(R_{n\ell})\right) + \frac{2mr^2}{\hbar^2}(E - V(r)) =$$

$$\frac{-1}{Y_{\ell m}}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}(Y_{\ell m})\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}(Y_{\ell m})\right]$$

$$= \lambda \quad , \text{Let } \lambda = \ell(\ell+1)$$

→ Radial part of schrodinger Eq

$$\frac{1}{R_{n\ell}} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} R_{n\ell}\right) + \frac{2mr^2}{\hbar^2}(E - V(r)) = \ell(\ell+1)$$

$$\Rightarrow \frac{\hbar^2}{2mr^2}\left[\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}(R_{n\ell})\right)\right] + (E - V(r)) R_{n\ell}$$

$$= \frac{\ell(\ell+1)\hbar^2}{2mr^2} R_{n\ell}$$

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(b) $\frac{\hbar^2}{2mr^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}(R_{nl})\right)\right] - R_{nl}\left(V(r) + \frac{l(l+1)\hbar^2}{2mr^2}\right)$

$$= -E R_{nl}$$

multiplying both sides by -1

$$\Rightarrow \frac{-\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}(R_{nl})\right) + R_{nl} V_{eff}(r)$$

$$= E R_{nl}(r) \quad -(2)$$

where $V_{eff}(r) = \frac{-e^2}{4\pi\varepsilon_0 r} + \frac{l(l+1)\hbar^2}{2mr^2}$

Taking $R_{nl}(r) = \frac{u_{nl}(r)}{r}$

$$\frac{\partial}{\partial r}(R_{nl}) = \frac{\partial}{\partial r}\left(\frac{1}{r}\cdot u_{nl}(r)\right) = \frac{1}{r}\frac{\partial}{\partial r}(u_{nl}) - \frac{1}{r^2}u_{nl}$$

$$r^2\frac{\partial}{\partial r}(R_{nl}) = r\frac{\partial}{\partial r}(u_{nl}) - u_{nl}$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}(R_{nl})\right) = \frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}(u_{nl}) - u_{nl}\right)$$

$$= \frac{\partial}{\partial r}(u_{nl}) + r\frac{\partial^2}{\partial r^2}(u_{nl}) - \frac{\partial}{\partial r}(u_{nl})$$

$$= r\frac{\partial^2}{\partial r^2}(u_{nl})$$

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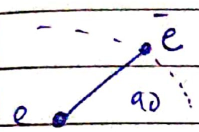
eq (2) in terms of $u_{nl}(r)$:

$$= -\frac{\hbar^2}{2m}\frac{1}{r^2}\left(r\frac{d^2}{dr^2}(u_{nl})\right) + \frac{u_{nl}}{r}V_{eff}(r) = \frac{u_{nl}(r)}{r}E$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dr^2}(u_{nl}) + u_{nl}V_{eff}(r) = u_{nl}(r)E \quad -(3)$$

rescaling r by a_0 (Bohr's Radius)



$$\frac{mv^2}{a_0} = \frac{e^2}{4\pi\varepsilon_0 a_0^2} \quad (i)$$

[centripetal force provided by coloumb force]

$$mva_0 = \hbar \quad (ii)$$

By (i) and (ii)

$$\frac{m\cdot\hbar^2}{m^2 a_0^2\cdot a_0} = \frac{e^2}{4\pi\varepsilon_0 a_0^2}$$

$$\Rightarrow a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$$

Let $r' = \frac{r}{a_0}$ where a_0

writing (3) in terms of r'

$$\frac{dr'}{dr} = \frac{1}{a_0}, \quad \frac{du}{dr} = \frac{du}{dr'}\cdot\frac{dr'}{dr}$$

$$\Rightarrow \frac{du}{dr} = \frac{du}{dr'}\cdot\frac{1}{a_0}$$

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$$\frac{d^2u}{dr^2} = \frac{d}{dr}\left(\frac{du}{dr}\right)$$

$$= \frac{1}{a_0}\frac{d}{dr}\left(\frac{du}{dr'}\right)$$

$$= \frac{1}{a_0}\frac{d}{dr'}\left(\frac{du}{dr}\right)$$

$$= \frac{1}{a_0}\frac{d}{dr'}\left(\frac{du}{dr'}\cdot\frac{1}{a_0}\right)$$

$$= \frac{1}{a_0^2}\frac{d^2u}{dr'^2}$$

$$u_{nl}(r) = u_{nl}(r')$$

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$$V(\text{eff})(r) = V(r) + \frac{l(l+1)\hbar^2}{2mr^2}$$

$$= \frac{-e^2}{4\pi\varepsilon_0 r} \cdot e^{-r/a} + \frac{l(l+1)\hbar^2}{2m(a_0 r')^2}$$

$$= \frac{-e^2}{4\pi\varepsilon_0 a_0 r'} e^{-\frac{r' a_0}{a}} + \frac{l(l+1)\hbar^2}{2m(a_0 r')^2}$$

Put value of a_0

$$V_{eff}(r') = \frac{me^4}{(4\pi\varepsilon_0)^2 \hbar^2}\left[-\frac{1}{r'} \cdot e^{-\frac{r' a_0}{a}} + \frac{l(l+1)}{2(r')^2}\right]$$

energy of ground state,

$$|E_1| = \frac{me^4}{2\hbar^2 (4\pi\varepsilon_0)^2}$$

eq. becomes:

$$\frac{-d^2}{d(r')^2} u_{nl}(r') + 2\left[-\frac{1}{r'} e^{-\frac{r' a_0}{a}} + \frac{l(l+1)}{2(r')^2}\right] u_{nl}(r')$$

$$= u_{nl}(r')\, E\left(\frac{2(4\pi\varepsilon_0)^2 \hbar^2}{me^4}\right)$$

dimensionless energy

$$\epsilon = \frac{E}{|E_1|}$$

dimensionless potential

$$V = \left[-\frac{2}{r'} e^{-\frac{r' a_0}{a}} + \frac{l(l+1)}{(r')^2}\right]$$

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take $l = 0$

$$V = \left[\frac{-2}{r'} e^{-\frac{r' a_0}{a}} \right]$$

$a_0 \rightarrow$ bohr radius

Let $r' = \xi$

$$\boxed{V = \left[\frac{-2}{\xi} e^{-\frac{\xi a_0}{a}} \right]}$$

Eq.:

$$\boxed{-\frac{d^2}{d\xi^2} K_{nl}(\xi) + V K_{nl}(\xi) = e K_{nl}(\xi)}$$

(c) Done in code and Discussion.

Programming

```
from scipy.linalg import eigh
import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import simps
import pandas as pd


def matrix_formation(a, b, N, f, alpha):

    x_range = np.linspace(a, b, N+2)
    h = x_range[1] - x_range[0]

    X = x_range[1: -1]
    g = f(X, alpha)

    l = np.zeros(len(X))
    d = np.zeros(len(X))
    u = np.zeros(len(X))

    for i in range(0, len(X)):
        d[i] = -(-2/h**2) - 1*g[i]
        l[i] = -(1/h**2)
        u[i] = -(1/h**2)

    diagonal = np.diag(d, k = 0)
    off_diag_l = np.diag(l[:-1], k = -1)
    off_diag_u = np.diag(u[:-1], k = 1)

    matrix = diagonal + off_diag_l + off_diag_u

    return matrix, X

def pot_col(x, alpha):
    potential = []
    for j in x:
            val = 2*((1/j))
            potential.append(val)

    return potential

def pot_screen(x, alpha):
    potential = []
    for j in x:
            val = 2*((1/j)*np.exp(-j/alpha))
            potential.append(val)

    return potential


def normalize(x, u):
    return u/np.sqrt(simps(u**2, x))

def V_r(x):

    return -2/x

def V_screening(x, alpha):

    return (-2/x)*np.exp(-x/alpha)


r_range = np.linspace(0.1, 2, 500)
alpha_vals = [2, 5, 10, 20, 100]

plt.plot(r_range, V_r(r_range), label = 'V(Coulomb) for l=0 ')
```

```
for i in alpha_vals:
    plt.plot(r_range, V_screening(r_range, i), label = f'V(screening) for alpha = {i}')

plt.title('Potential Plots')
plt.xlabel(r"$\xi$")
plt.ylabel("V")
plt.legend()
plt.grid()
plt.show()

ground_state_vals = []

for i in alpha_vals:

    matrix, X = matrix_formation(0, 200, 1000, pot_screen, i)
    e , vec = eigh(matrix)

    print(f'Energy Eigen Values(alpha={i}) = ', e[:5])

    ground_state_vals.append(e[0])


ground_state_energy = np.multiply(ground_state_vals, 13.6)

data = {

  'alpha': alpha_vals,
  'Ground_State_Energy(eV)': ground_state_energy

}

df = pd.DataFrame(data)
print(df)


x_range = np.linspace(0, 20, 1000)

matrix1, X1 = matrix_formation(0, 20, 1000, pot_col, 0)
e1 , vec1 = eigh(matrix1)
norm1 = normalize(X1, vec1.T[0])

plt.scatter(X1, norm1,s = 5, label = 'Coulomb Potential')

for i in alpha_vals:

    matrix2, X2 = matrix_formation(0, 20, 1000, pot_screen, i)
    e2 , vec2 = eigh(matrix2)
    norm2 = normalize(X2, vec2.T[0])
    plt.plot(X2, norm2, label = f'Screening Potential for alpha = {i}')

plt.title('Ground State WaveFunction')
plt.xlabel(r"$\xi$")
plt.ylabel("K_nl")
plt.legend()
plt.grid()
plt.show()


matrix1, X1 = matrix_formation(0, 20, 1000, pot_col, 0)
e1 , vec1 = eigh(matrix1)
norm1 = normalize(X1, vec1.T[0])

plt.scatter(X1, norm1**2,s = 5, label = 'Coulomb Potential')

for i in alpha_vals:

```

```
    matrix2, X2 = matrix_formation(0, 20, 1000, pot_screen, i)
    e2 , vec2 = eigh(matrix2)
    norm2 = normalize(X2, vec2.T[0])
    plt.plot(X2, norm2**2, label = f'Screening Potential for alpha = {i}')

plt.title('Ground State Probability Density')
plt.xlabel(r"$\xi^2$")
plt.ylabel("K_nl")
plt.legend()
plt.grid()
plt.show()

plt.plot(alpha_vals, ground_state_energy)
plt.scatter(alpha_vals, ground_state_energy, color ="red")
plt.title('Ground State Energy Vs Alpha')
plt.xlabel(r"Alpha")
plt.ylabel("E0(eV)")
plt.grid()
plt.show()
```

Result and Discussion

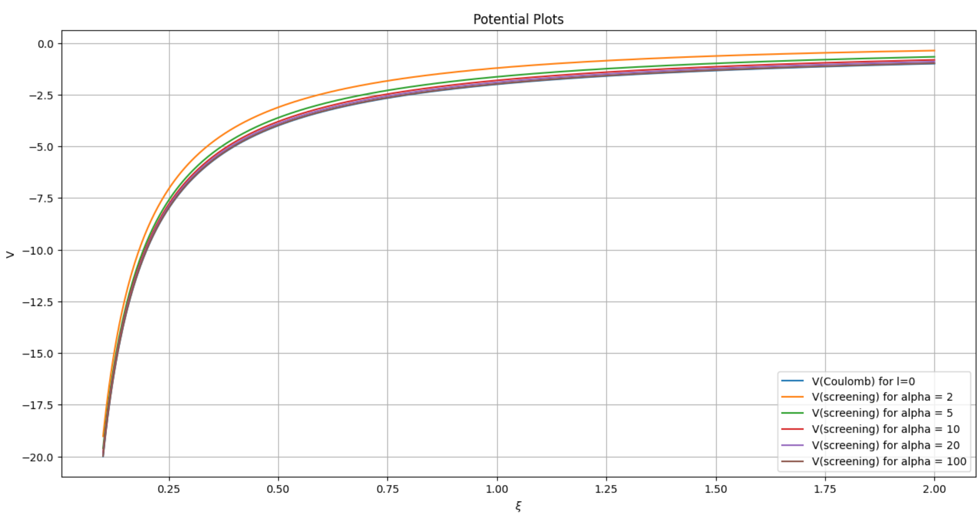

Figure 1: Potential Plots

It can be seen that as the value of alpha goes on increasing the screening potential approaches the coulomb potential.

```
Energy Eigen Values(alpha=2) =  [-2.88282673e-01  2.50378573e-04  1.00161822e-03  2.25401620e-03
  4.00802272e-03]
Energy Eigen Values(alpha=5) =  [-6.44164957e-01 -2.38633586e-02  2.73217297e-04  1.09286655e-03
  2.45850699e-03]
Energy Eigen Values(alpha=10) =  [-8.04420603e-01 -9.93092588e-02 -6.35896479e-03  3.11183804e-04
  1.24730025e-03]
Energy Eigen Values(alpha=20) =  [-8.93870908e-01 -1.62942216e-01 -3.86000697e-02 -6.16096121e-03
  1.08212757e-04]
Energy Eigen Values(alpha=100) =  [-0.97036434 -0.22996686 -0.09227568 -0.04467415 -0.02330694]
```

Figure 2: Eigen Value Variation with Alpha

There are finite number of bound states. It can be seen that the Eigen values for higher values of n becomes positive which physically does not equate to a bound state. As we increase the value of alpha the number of bound states go on increasing.

	alpha	Ground_State_Energy(eV)
0	2	-3.920644
1	5	-8.760643
2	10	-10.940120
3	20	-12.156644
4	100	-13.196955

Figure 3: Ground State Energy Variation with Alpha

It can be seen that as the value of alpha increases the ground state energy approaches the ground state energy for coulomb potential(-13.6eV).

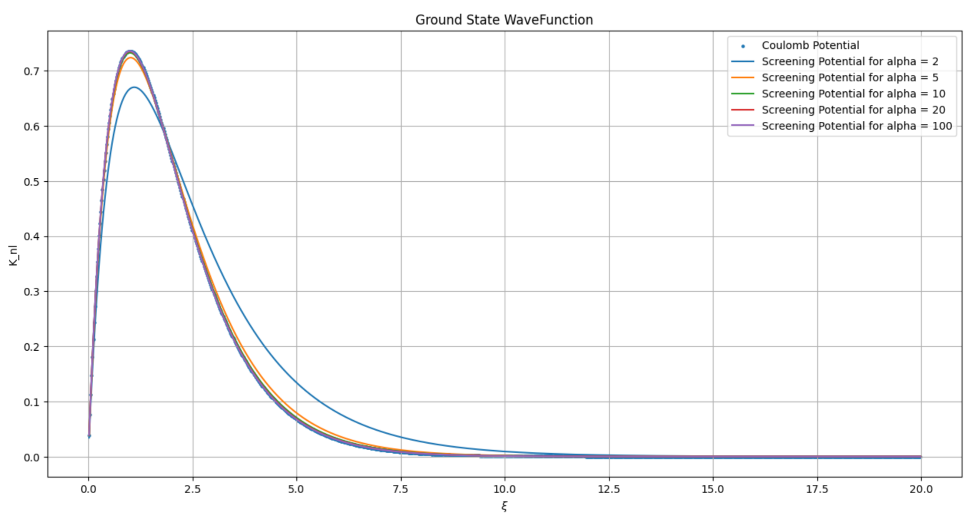

Figure 4: Ground State Wave Functions

This is the ground state wavefunction, it can be seen that for smaller values of alpha graph shows variation but as we approach higher values of alpha the lines start to coincide with the coulomb potential.

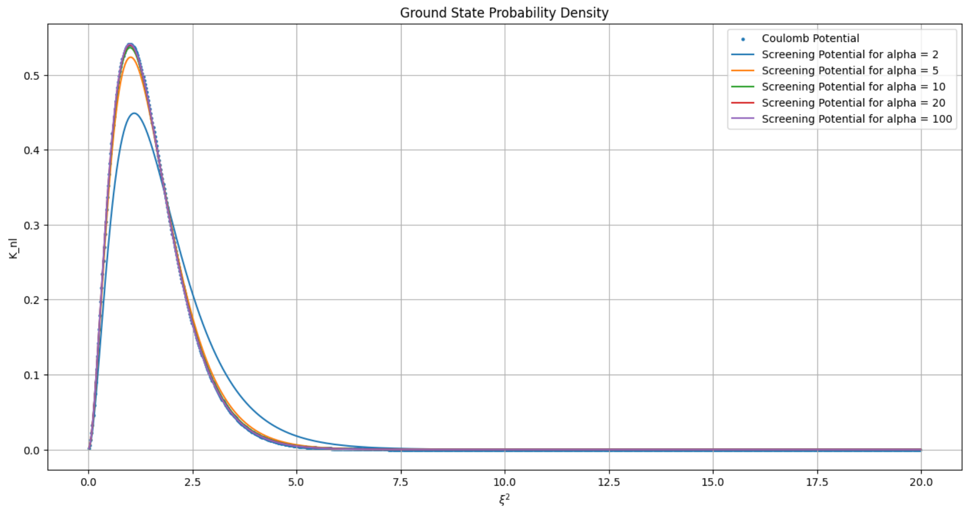

Figure 5: Ground State Probability Densities

A similar observation can be seen for the probability density as for the wavefunction.

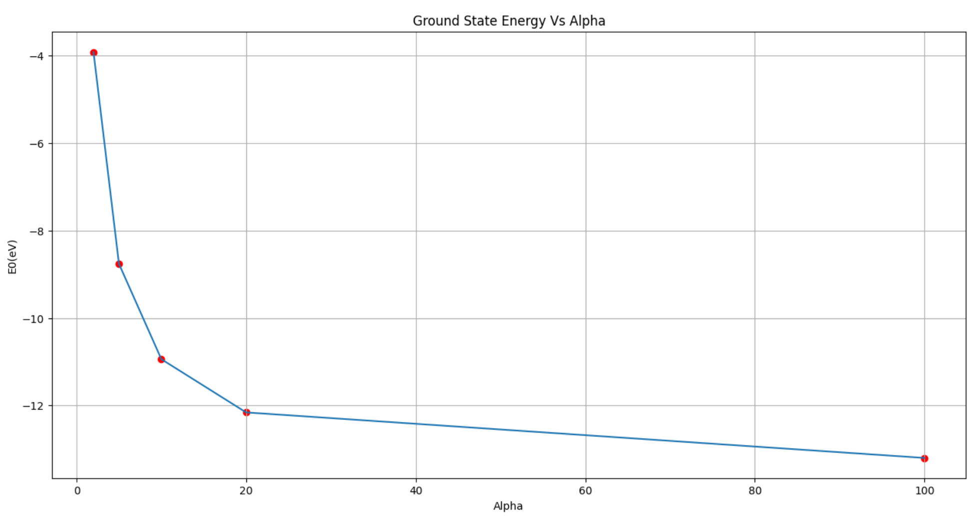

Figure 6: Ground State Energy as a function of Alpha

It can be seen that as we increase the value of alpha the ground state energy approaches the ground state energy for coulomb potential(-13.6eV).