Assignment 5 - Harmonic Oscillator - I

SGTB Khalsa College, University of Delhi

Ankur Kumar(2020PHY1113)(20068567010)

Unique Paper Code: 32221501

Paper Title: Quantum Mechanics

Submitted on: August 22, 2022

B.Sc(H) Physics Sem V

Submitted to: Dr. Mamta

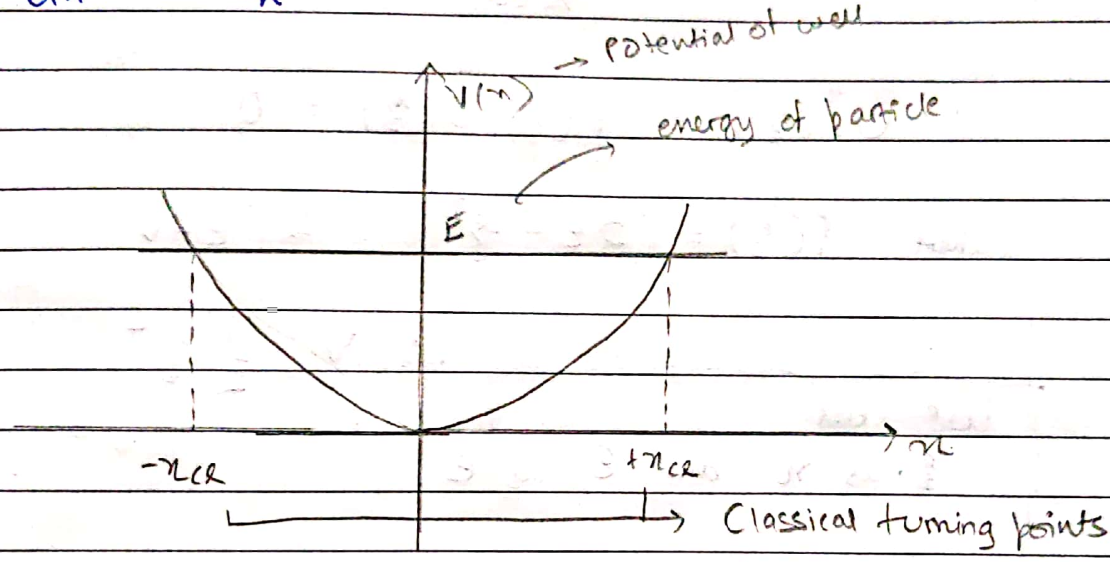
Date

Theory:

Particle mass 'm'

Potential $V(x) = \frac{1}{2} m\omega^2 x^2$.

(a) $$\frac{d^2 u}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2} m\omega^2 x^2\right) u(x) = 0$$



define $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$

and $\xi_{cl} = \sqrt{\frac{m\omega}{\hbar}}\, x_{cl} = 1$

$$\frac{d}{dx} = \sqrt{\frac{m\omega}{\hbar}}\frac{d}{d\xi} \qquad \frac{d^2}{dx^2} = \frac{m\omega}{\hbar}\frac{d^2}{d\xi^2}$$

→ Put in eq.

$$-\frac{\hbar^2}{2m}\cdot\frac{m\omega}{\hbar}\frac{d^2 u}{d\xi^2} + \frac{1}{2} m\omega^2\left(\frac{\hbar}{m\omega}\right)\xi^2 = E\,u$$

Page No.
Date

$$-\frac{\hbar\omega}{2}\frac{d^2 U}{d\xi^2} + \frac{\hbar\omega}{2}\xi^2 = EU$$

$$\frac{d^2 U}{d\xi^2} - \xi^2 U = -\frac{2E}{\hbar\omega} \cdot U$$

Let $\varepsilon = \frac{E}{\hbar\omega}$ $\{\omega \to \text{freq.}\}$

$$U''(\xi) + f(\xi)\, U(\xi) = 0$$

where, $f(\xi) = (2\varepsilon - \xi^2) = 2(\varepsilon - V)$

$\therefore V = \frac{1}{2}\xi^2$

We call,
ξ as x and ε as e,

$U''(x) + f(x)\, U(x) = 0$; $f(x) = 2(e - V(x))$

$V(x) = \frac{1}{2}x^2$

(b) The energy eigen values come out to be:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

The classical turning points, are those points where the total energy of the particle gets converted into the potential energy.

$$E_n = V(x)$$

$$\left(n+\frac{1}{2}\right)\hbar \cancel{\omega} = \frac{1}{2} m \omega^{2} x_{cl}^{2}$$

$$\cancel{2}\cdot\left(\frac{2n+1}{\cancel{2}}\right)\frac{\hbar}{m\omega} = x_{cl}^{2}$$

$$\boxed{x_{cl} = \pm\sqrt{(2n+1)\frac{\hbar}{m\omega}}}$$

we know,

$$\xi = \sqrt{\frac{m\omega}{\hbar}}\cdot x$$

$$\therefore \quad \boxed{\xi_{cl} = \sqrt{2n+1}} \qquad n = 0, 1, 2, 3 \ldots\ldots$$

→ Dimensionless form for classical turning points.

we know, that $\varepsilon = \dfrac{E}{\hbar\omega} \Rightarrow E_n = \varepsilon_n \cdot \hbar\omega$

$$\therefore \quad \varepsilon_n \cdot \cancel{\hbar\omega} = \left(n+\frac{1}{2}\right)\cancel{\hbar\omega}$$

$$\boxed{\varepsilon_n = \left(n+\frac{1}{2}\right)}$$

→ Dimensionless form for energy eigen values.

(c) Let $\alpha = \dfrac{m\omega}{\hbar}$, $\therefore \xi = \sqrt{\alpha}\, x$

Page No.
Date

(c) $$U_n(\xi) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)\, e^{-\xi^2/2}$$

where $H_n(\xi) \rightarrow$ Hermite polynomial

$$\psi_0 = \left(\frac{\alpha}{\pi}\right)^{1/4} \cdot e^{-\xi^2/2}$$

$$U_1 = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2}\,\xi\, e^{-\xi^2/2}$$

$$U_2 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} (2\xi^2 - 1)\, e^{-\xi^2/2}$$

$$U_3 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}} (2\xi^3 - 3\xi)\, e^{-\xi^2/2}$$

$$U_4 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{2\sqrt{6}} (4\xi^4 - 12\xi^2 + 3)\, e^{-\xi^2/2}$$

(d) <u>Non-zero value of ground state Energy</u>

we know, by Heinsberg's relⁿ, $\Delta p \cdot \Delta x \approx \hbar$

Particle confined in a box/well, so $\Delta x \sim a$ — dimension of well

$$\therefore \Delta p \approx \frac{\hbar}{a}$$

$$\therefore E_{min} \approx \frac{(\Delta p)^2}{2m} \approx \frac{\hbar^2}{2ma^2}$$

$\therefore$ Even in the lowest state, the particle must have some energy so as to obey Heisenberg's relⁿ, $\longrightarrow$ <u>Zero point Energy</u>

Programming

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

def f(x, e):
    return 2*(e - (1/2)*(x**2))

def e(n, delta = 0):
    return n + (1/2) + delta

def numerov(func, u0, x_max, points, e, n, delta):

    x_range = np.linspace(0, x_max, points)
    h = x_range[1] - x_range[0]
    u_values = np.zeros(len(x_range))
    u_values[0] = u0

    c_values = np.ones(len(x_range)) + np.multiply((h**2)/12, func(x_range, e(n, delta)))

    if u0 == 0:
        u_values[1] = u0 + h
    else:
        u_values[1] = ((6 - 5*c_values[0])/c_values[1])*u0


    for i in range(1, len(x_range)-1):
        u_values[i+1] = (1/c_values[i+1])*((12-10*c_values[i])*u_values[i] - c_values[i-1]*u_values[i-1])

    extended_u = []

    if u0 == 0:

        for i in range(1, len(x_range)):
            extended_u.append(-1*(u_values[-i]))

        for i in range(0, len(x_range)):
            extended_u.append(u_values[i])

    else:
        for i in range(1, len(x_range)):
            extended_u.append(1*(u_values[-i]))

        for i in range(0, len(x_range)):
            extended_u.append(u_values[i])

    extended_u = np.array(extended_u)

    extended_x_vals = np.linspace(-x_max, x_max, 2*points-1)

    norm = (simps((extended_u)**2, extended_x_vals))
    u_list = (extended_u)/np.sqrt(norm)


    return extended_x_vals, u_list

delta_e = [1e-2, 1e-4, 1e-6, 1e-8]

#Ground State
for i in range(0, len(delta_e)):
    x_vals, result = numerov(f, 1, np.sqrt(1), 100, e, 0, delta_e[i])
    plt.scatter(x_vals, result, label = f'delta_e_{i}', s = 5)

```

```
x_vals_analyitc, result_analytic = numerov(f, 1, np.sqrt(1), 100, e, 0, 0)
plt.plot(x_vals_analyitc, result_analytic, label = 'Analytical Solution')
plt.title('Ground State - Variation of Delta_e')
plt.xlabel(r'$\xi$')
plt.ylabel(r'$U(\xi)$')
plt.grid()
plt.legend()
plt.show()

#First Three Excited States
initial_conds = [0, -1]
for i in range(1, len(initial_conds)+1):

    x_vals, result = numerov(f, initial_conds[i-1], np.sqrt(2*i+1), 100, e, i, 1e-6)
    plt.scatter(x_vals, result, label = 'Numerov Solution', s = 10, color = 'red')
    x_vals_analytic, result_analytic = numerov(f, initial_conds[i-1], np.sqrt(2*i+1), 100, e, i, 0)
    plt.plot(x_vals_analytic, result_analytic, label = 'Analytical Solution')

    plt.title(f'N = {i} ')
    plt.xlabel(r'$\xi$')
    plt.ylabel(r'$U(\xi)$')
    plt.legend()
    plt.grid()
    plt.show()


x_vals, result = numerov(f, 0, np.sqrt(7), 100, e, 3, 1e-6)
plt.scatter(x_vals, -1*result, label = 'Numerov Solution', s = 10, color ='red')
x_vals_analytic, result_analytic = numerov(f, 0, np.sqrt(7), 100, e, 3, 0)
plt.plot(x_vals_analytic, -1*result_analytic, label = 'Analytical Solution')

plt.title('N = 3')
plt.xlabel(r'$\xi$')
plt.ylabel(r'$U(\xi)$')
plt.legend()
plt.grid()
plt.show()

#Probability Densities

initial_conds = [1, 0, -1]
for i in range(0, len(initial_conds)):

    x_vals, result = numerov(f, initial_conds[i], np.sqrt(2*i+1), 100, e, i, 1e-6)
    plt.scatter(x_vals, result**2, label = f'Numerov Solution N = {i}', s = 10, color = 'red')
    x_vals_analytic, result_analytic = numerov(f, initial_conds[i], np.sqrt(2*i+1), 100, e, i, 0)
    plt.plot(x_vals_analytic, result_analytic**2, label = f'Analytical Solution N = {i}')


x_vals, result = numerov(f, 0, np.sqrt(7), 100, e, 3, 1e-6)
plt.scatter(x_vals, (-1*result)**2, label = f'Numerov Solution N = 3', s = 10, color ='red')
x_vals_analytic, result_analytic = numerov(f, 0, np.sqrt(7), 100, e, 3, 0)
plt.plot(x_vals_analytic, (-1*result_analytic)**2, label = f'Analytical Solution N = 3')

plt.title('Probability Densities')
plt.xlabel(r'$\xi$')
plt.ylabel(r'|$U^2(\xi)$|')
plt.legend()
plt.grid()
plt.show()
```

```python

#Energy Values

def energy(n, omega, delta = 0):

    e = 1.6e-19
    h_cut =  1.05457182e-34
    return ((n + 1/2 + delta) * h_cut * omega)/e

energy_calc = []
energy_analytic = []
n = []

for i in range(0,4):
    energycalc = energy(i, 5.5e14, delta = 1e-6)
    energy_calc.append(energycalc)

    energyanalytic = energy(i, 5.5e14, delta = 0)
    energy_analytic.append(energyanalytic)

    n.append(i)

data = {

  'n': n,
  'Calculated Energies(eV)': energy_calc,
  'Analytical Energies(eV)': energy_analytic

}

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

#PROBABILITY

x_vals_prob, result_prob =  numerov(f, 1, np.sqrt(9), 150, e, 0, 0)

slice_x = x_vals_prob[99:200]
slice_result = result_prob[99:200]

Probability = simps((slice_result)**2, slice_x)

print('Probability = ', 1 - Probability)
```

Result and Discussion

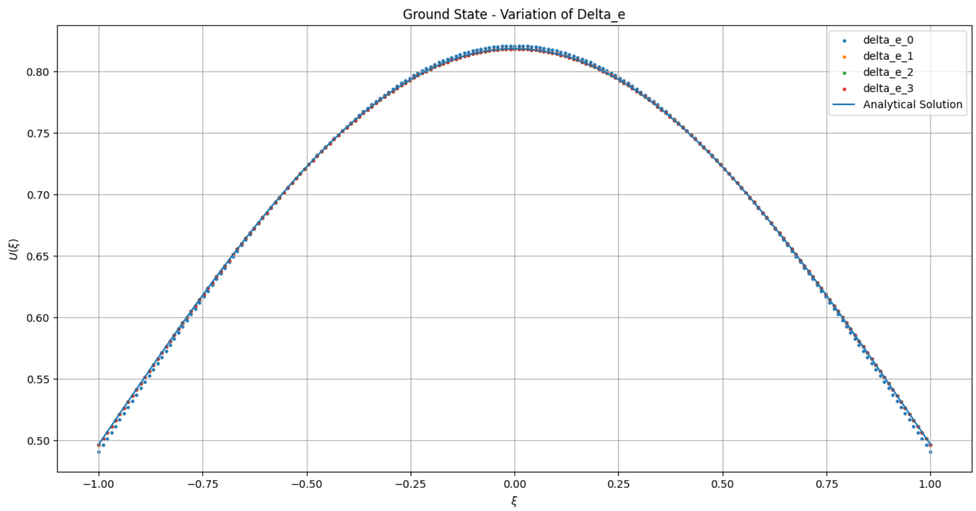


Figure 1: Delta e Variation - Ground State

This is the plot of the ground state with the variation of the Delta e. As the value of Delta e decreases the plot approaches the Analytical Solution.

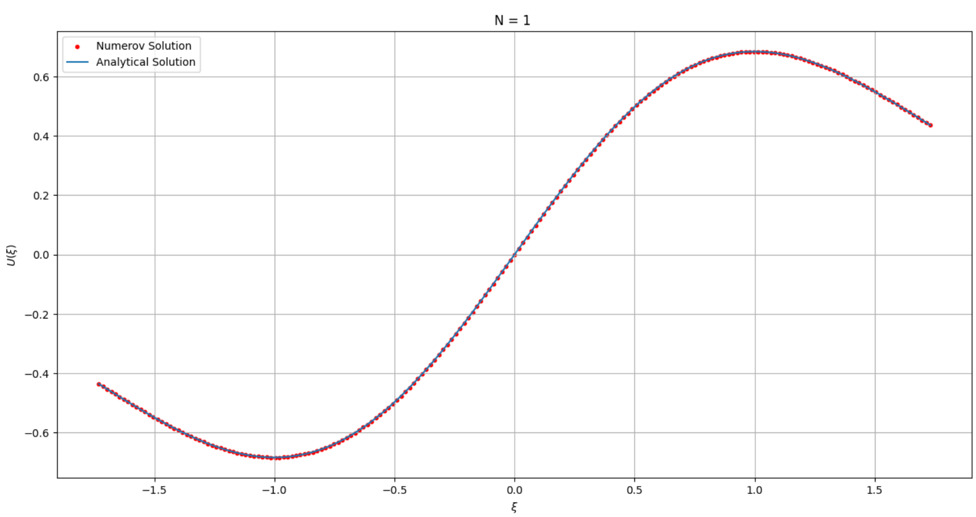


Figure 2: N=1

The First excited state.

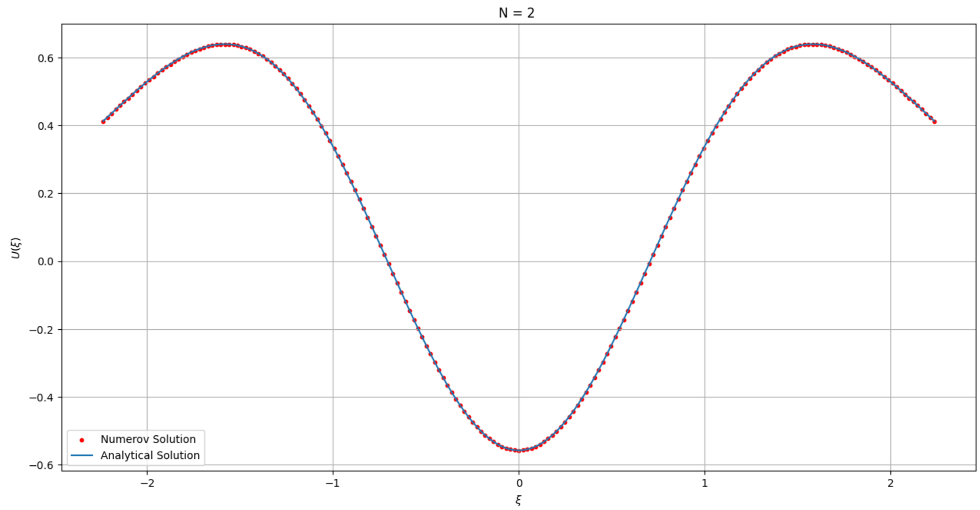


Figure 3: N=2

The Second excited state.

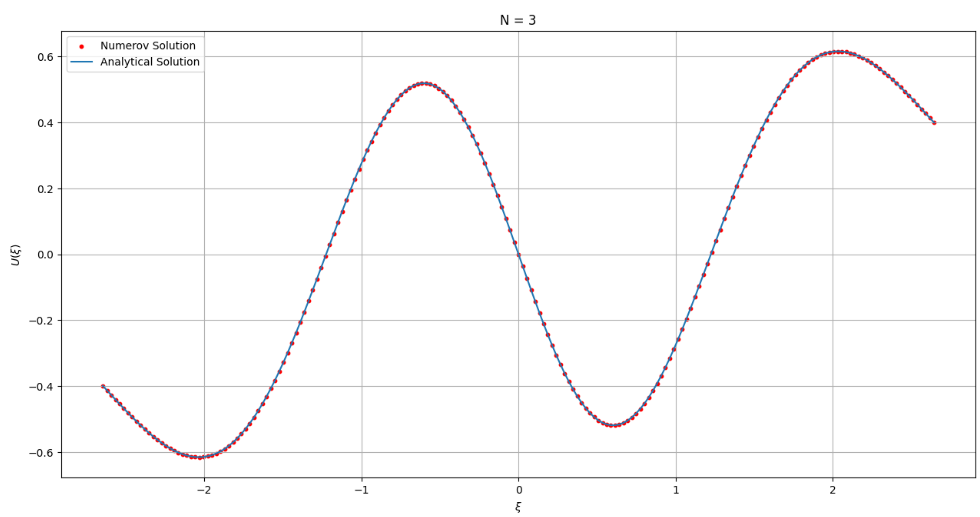


Figure 4: N=3

The Third excited state.
In all three figures, delta e is taken as 10^{-6}.

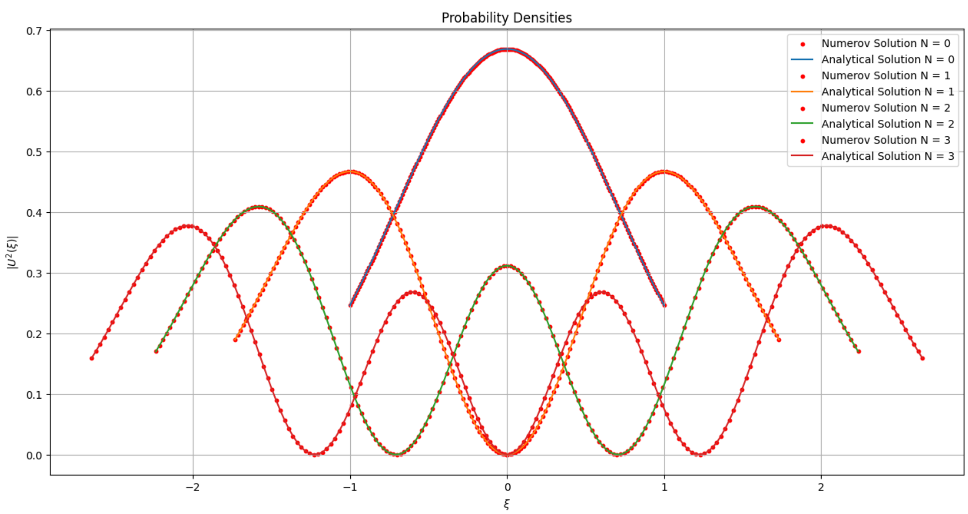


Figure 5: Probability Densities

The plot of the first 4 probability densities plotted together.

	n	Calculated Energies(eV)	Analytical Energies(eV)
0	0	0.181255	0.181255
1	1	0.543764	0.543764
2	2	0.906273	0.906273
3	3	1.268782	1.268782

Figure 6: Energy Eigen Values

The energy eigen values of the the first 4 states is given above along with their analytical values.

```
Probability =  0.1545132256585161
```

Figure 7: Probability

The probability of finding electron in the classically forbidden region when it is in the ground state.