Lab Assignment 11

June 2, 2021

The Schrödinger equation for the harmonic oscillator is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi \tag{1}$$

where

ω is the frequency of oscillation,
$\hbar$ is the Planck's constant,
m is the mass of the particle,
ψ is the particle's wave function, and
E is the energy, and is given by $E = \left(n + \frac{1}{2}\right)\hbar\omega$. ($n$=0,1,2,3,.... is an integer)

The analytical result is given by

$$\psi(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{\frac{-m\omega}{2\hbar}x^2} \tag{2}$$

Question:
Write a program to solve the differential equation given in equation (1) for the ground state (n=0). You should have the following components in your program:

a) Write a function to solve the differential equation using RK4 method in the range $x = -2.5$ to $x = 2.5$ with step size $h = 0.25$.

Initial conditions are

- $\psi(-2.5) = 0.03300$
- $\left.\frac{d\psi}{dx}\right|_{x=-2.5} = 0.08250$

b) Write a function to obtain the analytical result for different values of x.

c) Call the functions from step (a) and (b) in `main()` to obtain the RK4 and analytical solutions. Store the values of x, $\psi(x)$ (RK4) and $\psi(x)$ (analytical) in a file named "QHO.dat"

In this problem take $\hbar = m = 1.0$, $\omega = 1.0$ Hz

Format of the output :

x	$\psi(x)$ (RK4)	$\psi(x)$ (analytical)
-2.50	...	...
-2.25	...	...
.	...	...
.	...	...
2.50	...	...

Plot the analytical result along with the results obtained from RK4.