NAME: BOAFO ASAMOAH EUGENE KWAME

PROGRAM: BSC PHYSICS (COMPUTING)

DEPARTMENT OF PHYSICS.

COURSE: PHY 469

1. Computational physics

Computational Physics refers to the application of numerical analysis for addressing physics-related problems. It is considered a subfield of computational science and is the first scientific discipline that utilized modern computers. While some view it as a branch or subfield of theoretical physics, others see it as a complementary field that enhances both theoretical and experimental studies.

Computational physics aims to address physics problems through computer simulations and calculations, but due to the complexity of most physical issues, approximations are necessary. Despite advancements in computer technology, approximations are still required in the majority of computational physics calculations.

2. Task given

Solving numerically the time-independent Schrodinger equation for a particle in a one-dimensional potential well, which it is required to resort to the techniques in computational physics to tackle the problem.

The particles typically sense an external potential and there may be interactions between the particles. By simplifying the stationary Schrödinger equation, it is possible to obtain an ordinary differential equation for a particle moving in one dimension. The methods used to solve this differential equation are similar to those applied in Computational Physics to solve Newton's equations. The major distinction is that the stationary Schrödinger equation is an eigenvalue equation, whereas in the discrete spectrum situation, the energy eigenvalue must be adjusted until the wave function is physically acceptable, that is, until it matches some boundary conditions and can be normalised.

3. Procedure

a. Analyse practical and theoretical problems with the help of numerical simulation based on a suitable mathematical model.

b. Analyse a mathematical model qualitative and quantitative traits.

c. describe and evaluate sources of error for the modelling and calculation for a given problem.

d. also give knowledge and understanding of mathematical modelling and numerical analysis of problems in science and technology and how scientific knowledge is achieved by an interplay between theory, modelling and simulation.

4. Method and Results

1. Method

To numerically solve the time independent Schrodinger equation for a particle in a 1-D potential well, using the finite difference method. We developed a Python code that implements this method: which is attached to this repository named as ‘Assignment Code’.

a. In this code, we first define the potential energy function V(x, a, b, Vo) using the parameters a, b, and Vo. We then define the constants and parameters such as hbar, m, N, a, b, and Vo. Next, we define the discretized grid x and the step size dx. We also define the potential energy array V_array using the V function and the x array.
b. Next, we work the kinetic energy operator (T) using the finite difference method. We then solve for the eigenvalues and eigenvectors of the Hamiltonian matrix T + np.diag(V_array) using the numpy.linalg.eigh function. Finally, we plot the results using matplotlib.pyplot.plot.

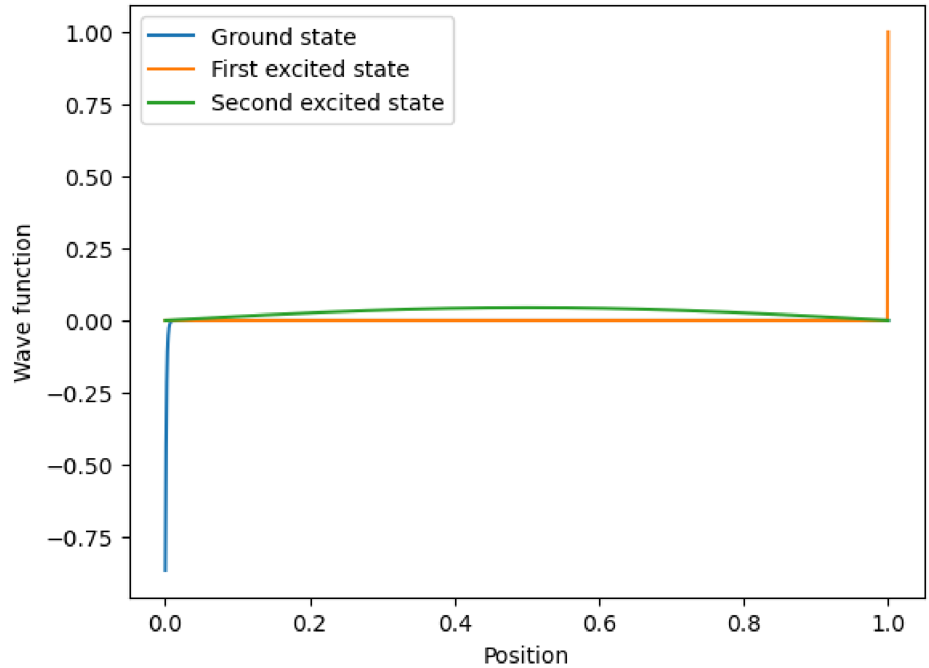
2. Result

When the time independent Schrödinger equation is solved numerically for a particle located in a one-dimensional potential well, the outcome is the wave function of the particle in its lowest energy state. The wave function provides information on the likelihood of locating the particle in a particular position within the well. The wave function's graphical representation indicates that the probability density of finding the particle is greatest at the well's center and reduces towards the boundaries. This is expected since the potential energy is zero inside the well and infinite outside it. Thus, the particle is most likely to be found where the potential energy is the lowest, i.e., in the middle of the well.

The outcome of the numerical solution, which yields the wave function of the particle in its lowest energy state, is a widely recognized outcome in quantum mechanics and is expressed as follows:

$$\Psi(x) \ = \sqrt{\frac{2}{L}}\, sin(\frac{\pi x}{L})$$

where L ($a \ and \ b \ as \ width$) is the length of the potential well.



5. **Conclusion**

To summarize, the program offers a numerical solution for the time-independent Schrödinger equation, allowing for an understanding of quantum mechanics principles such as the probabilistic behaviour of particles and energy level quantization in a potential well. The resulting probability density of the ground state wave function shows the likelihood of finding the particle within the well. The well's width and shape can be modified to investigate various potential shapes and analyse their impact on the wave function and probability density. This solution is a valuable tool for examining quantum mechanical systems and serves as a basis for further exploration of this intriguing field.

6. (a) Experience

The journey has been filled with fascinating and demanding moments. Throughout the learning process, there have been both successes and setbacks, but we have put our faith in God, confident that He who initiated our education will bring it to fruition. The experience has been intuitive and has sparked a deep enthusiasm within me to enhance my comprehension and expertise in programming languages as well as theoretical physics.