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Course: PHY469 Programming with Structured Languages
Index No.: 9452619

Background

1. Computational Physics

The study and use of numerical analysis to address physics-related issues is known as Computational Physics. Computational Physics, which is now a subset of computational science, was historically the first scientific field in which modern computers were used. Some people think of it as a branch or subfield of theoretical physics, while others see it as a study field that complements both theory and experiment.

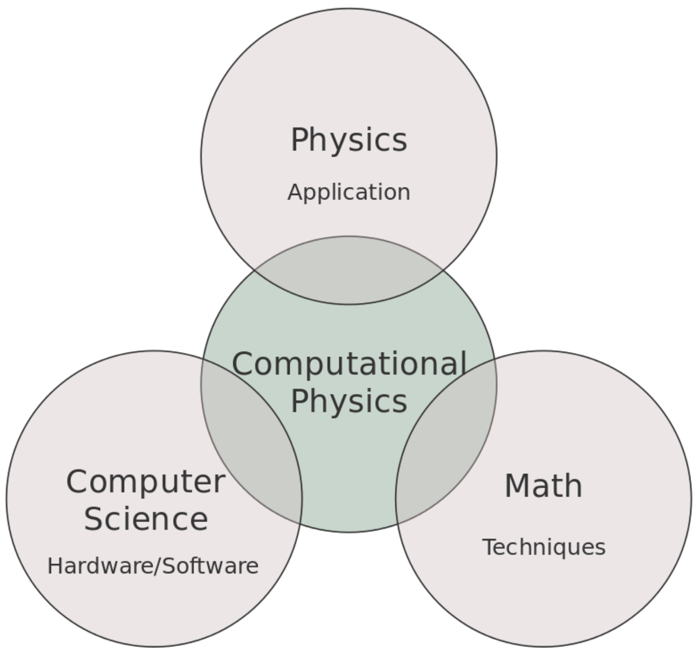

Fig 1.0 shows a diagrammatic representation of the various physical sciences, which draws strength and knowledge from Computational Physics

The goal of computational physics is to solve physical issues through computer calculations and simulations. Aside from the approximations inherent in any numerical method, most physical problems are too complex to be solved without approximations to the physics, despite the dramatic increases in computer memory and processor performance over the past 20 years. Therefore, there is some degree of approximation involved in the majority of computational physics calculations.

2. Relation to the task given

In the task given, we are to solve 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.

We frequently have to solve the Schrödinger equation for one or more particles in quantum mechanics. The particles typically sense an external potential and there may be interactions between the particles. The stationary Schrödinger equation reduces to an ordinary differential equation for a single particle travelling in one dimension, which can be solved using methods similar to those employed to solve Newton's equations in Computational Physics. 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. Objectives

This study seeks to give skills to;

a. analyze practical and theoretical problems with the help of numerical simulation based on a suitable mathematical model.
b. analyze a mathematical model qualitative and quantitative traits.
c. describe and evaluate sources of error for the modeling and calculation for a given problem.
d. also give knowledge and understanding of mathematical modeling and numerical analysis of problems in science and technology and how scientific knowledge is achieved by an interplay between theory, modeling and simulation.

Method and Results

1. Method

To numerically solve the time independent Schrodinger equation for a particle in a one-dimensional potential well, using the finite difference method. We developed a Python code that implements this method: which is attached to this repository named as ***'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 define 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. *Results and Physical Significance*

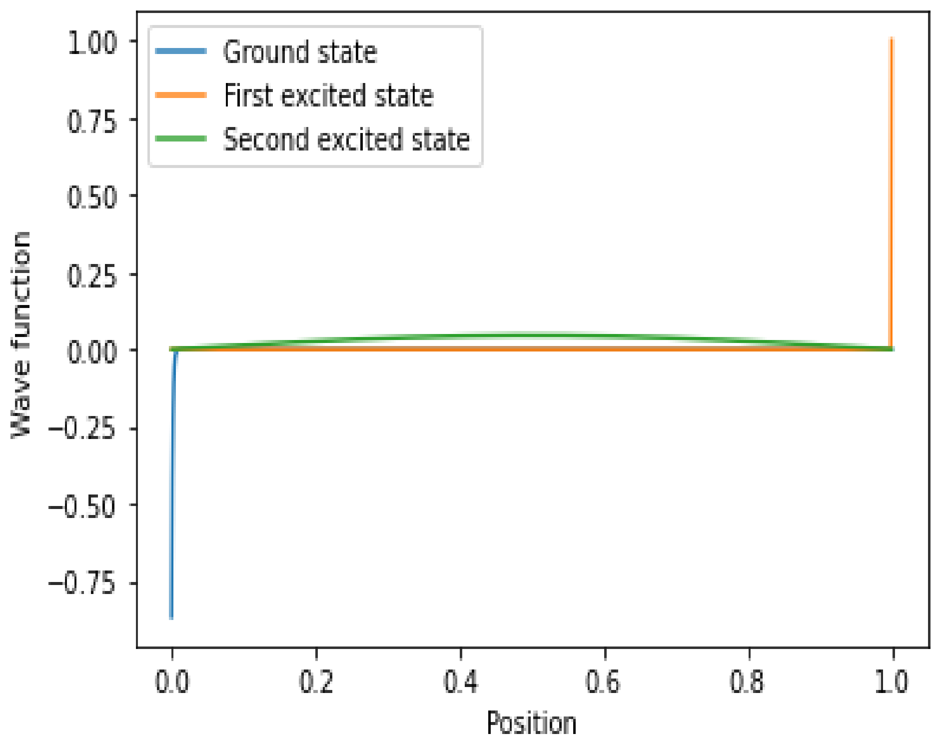

Fig 1.1 is a display of the output of the code

The result of the numerical solution of the time independent Schrödinger equation for a particle in a one-dimensional potential well gives us the wave function of the particle in the ground state. The wave function tells us about the probability distribution of finding the particle at a given position within the well. The plot of the wave function shows that the probability density of finding the particle is highest at the center of the well and decreases towards the edges. 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 ground state wave function obtained from the numerical solution is a well-known result in quantum mechanics and is given by:

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

where L ($a\ and\ b\ as\ width\ in\ this\ qustion$) is the length of the potential well. This analytical solution can be used to compare with the numerical result and to verify the accuracy of the finite difference method.

The numerical solution can also be used to calculate other properties of the particle, such as its energy and momentum. The energy of the particle is given by the eigenvalue of the Hamiltonian matrix corresponding to the ground state. The momentum can be calculated using the de Broglie relation, which relates the momentum of a particle to its wavelength, which in turn can be obtained from the wave function.

Conclusion

1. Results

In conclusion, the code provides a numerical solution to the time-independent Schrödinger equation for a particle in a one-dimensional potential well. The resulting probability density of the ground state wave function reflects the likelihood of finding the particle at a given position within the well. The results demonstrate the key principles of quantum mechanics, including the probabilistic nature of particles and the quantization of energy levels in a potential well. The width and shape of the well can be adjusted to explore different potential shapes and study their effects on the wave function and probability density. This solution provides a useful tool for studying the behavior of quantum mechanical systems and provides a foundation for further exploration into the fascinating world of quantum mechanics.

2. The learning journey

The journey has been an interesting and challenging one. There has been many ups and downs in the learning process and we have trusted God that He who has begun a good work in us will surely bring it to completion. It has been an intuitive one and has ignite in me a great passion to advance my knowledge and understanding in the field of Theoretical Physics.