Proposal for semester project in Introductory Computational Physics Course

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1   Aim

Solving The Schrodinger equation with a known potential using numerical techniques.

2   Plan

Most of quantum problems are solved by using Schrodinger equation, but there are only few problems that can be solved exactly. The most notably are the harmonic oscillator, particle in a box and hydrogen atom. In this project I'll try to solve Schrodinger equation by using numerical techniques(those which can not be solved analytically).

Firstly I'll start with solving the exactly soluble problems(simple cases) in order to learn implementation of numerical techniques on the problems. Then I planned to go further and try some complex potentials(Lennard Jones, Yukawa etc.).I'll solve equation for eigen functions and energy eigen values.

3   Techniques used

At the first glance I can say that I'll use finite-difference forms of differential equations,the shooting and matching methods,verlet method, numerov method. If these will not be sufficient, then I can go for matrix approach to solve the problem. In last variational methods can also be used.

Instead of all these, I'll also make sure about the numerical instability and accuracy of the computation.