Curiosity Gym Project

Gaurav Goel

Mentor: Carl Rozario

Aim: To develop a software model on Python to predict numerically the helium atom spectrum using the Hartree-Fock method and to compare the results with experimental values.

Method:

1. Develop mathematical machinery required for calculations including matrix manipulations, polynomial algebra and thus calculation of eigenvalues of matrices numerically; and of numerical solutions to differential equations.
2. Apply this machinery to solve Schrödinger Equation for simple systems like an infinite potential well and parabolic potential well.
3. Use the Hartree-Fock method to solve the Schrödinger Equation for the hydrogen atom and then finally for the helium atom.

Progress Made: 1

Description of Method:

1. Polynomials are modeled by lists of their coefficients arranged in descending order of power. The functions pvalue (polynomial value at a given input), deriv (derivative of polynomial), polynr (approximate root of polynomial using Newton-Rhapson Method), allroots (all roots of the polynomial) and product (product of two polynomials) are implemented.
2. Matrices are modeled by multidimensional lists equipped with addition and mulitplication. Square matrices are implemented as a derived class of matrices equipped with an additional determinant operation.
3. Matrices with polynomial entries are used to calculate the eigenvalues of square matrices.
4. Simple first order and second order ODE’s are solved numerically. The implementation of a simple differential equation that produces the sine and cosine functions. Another application was to projectile motion and modeling bouncing of balls. This was elastic and inelastic collisions with the ground with given coefficient of restitution.
5. Some IVPs are solved using Euler’s method.

To be done:

To apply this machinery to solving the Schrödinger Equation for simple systems and then eventually to more complicated systems.