Project 2

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Abstract

The goal of this project is to explore a model of quantum dots. We will be investigating the behavior of two electron in a 3-D simple harmonic potential while comparing the models with and without the particles interacting. To do this we will be solving the Schrdinger equation using the Jacobi method.

1 Introduction

Finding the eigenvalues of a matrix can give information on properties of a system, such as energies or spin. These properties can be useful to know when experiments are performed. Since we can predict the Hamiltonian of a system using the Shrödinger equation. If we have a system with many particles, it is impractical to do so by hand, which is where computing eigenvalues from a matrix using computers becomes useful. Doing so will require a code that can find eigenvalues from a matrix, which is what the present work attempts to create.

1.1 Mathematical Motivation

The Hamiltonians that we will be concerned with will be in the form of a tridiagonal matrix and tridiagonal matricies are simple to get eigenvalues from, but if the matrix were 100x100, it would be too much to compute by hand.

2 Solution

2.1 Setup

We know that the hamiltonian is a tridiagonla matrix, where the diagonals are $2/\hbar^2$ +V_N and the elements on either side of the diagonals are -$1/\hbar^2$ for an NxN matrix:

$$H = \begin{bmatrix} \frac{2}{\hbar^2}+V_1 & -\frac{1}{\hbar^2} & 0 & 0 & ... & 0 \\ -\frac{1}{\hbar^2} & \frac{2}{\hbar^2}+V_2 & -\frac{1}{\hbar^2} & 0 & ... & 0 \\ 0 & -\frac{1}{\hbar^2} & \frac{2}{\hbar^2}+V_3 & -\frac{1}{\hbar^2} & ... & 0 \\ 0 & 0 & -\frac{1}{\hbar^2} & \frac{2}{\hbar^2}+V_4 & ... & 0 \\ ... & ... & ... & ... & ... & -\frac{1}{\hbar^2} \\ 0 & 0 & 0 & 0 & -\frac{1}{\hbar^2} & \frac{2}{\hbar^2}+V_{N-1} \end{bmatrix}$$

2.2 Jacobi Algorithm

2.3 Error

3 Conclusion

4 References