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:

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

This matrix is what we need to get the eigenvalues of. There is a function in python which tells us the eigenvalues of a matrix and we use this at the beginning of our code to see what eigenvalues to expect, so that once we create out Jacobi solver, we know whether the values returned are correct or not.

2.2 Jacobi Algorithm

2.3 Error

3 Conclusion

We have found that the Jacobi method is a slower way of finding the eigenvalues of a matrix compared to the built in eigenvalue solver function. But when we have large matricies, simply storing it could take up a significant amount of space, which is one of the downfalls of using the built in functions, they require a defined matrix to work, which may be impractical with a sufficiently large matrix. The Jacobi method is one solution to a matrix so large that it is not feasible to store it, where we can create a matrix using smaller vectors, while still being able to find reasonably close eigenvalues to what is returned from the built in functions.

4 References