Computational Physics - Project 2

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1 Introduction And Motivation

In many fields of both mathematics and physics, we often come to the point that we have to solve so-called eigenvalue problems, which are equations of the form $\hat{A} \cdot \hat{v} = \lambda \hat{v}$, where $\hat{A}$ is a matrix of dimension $n \times n$ and v is a vector of dimension n. Equations of this kind occur not only in linear algebra, but also in mechanics and quantum mechanics and will also be a major part of this report. In this project, we are going to rewrite the Schrödinger's equation of one and two electrons in a harmonic oscillator potential in the form of an eigenvalue problem and solve it numerically by implementing Jacobi's method, an algorithm that can be used to solve any eigenvalue problem.

2 Theory

2.1 Rewriting Schrödinger's equation as eigenvalue problem

2.1.1 One electron in a harmonic oscillator potential

2.1.2 Two interacting electrons in a harmonic oscialltor potential

2.2 Jacobi's method

3 Execution

3.1 Implementing the algorithm

3.2 Results

4 Comparison and discussion of the results