FYS3150-Project 2

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Abstract

1 Introduction

The aim of this project is solving eigenvalue/eigenvector problems using the Jacobi algorithm. Specifically, we will look at solving the Schroedinger's equation with a three-dimensional harmonic oscillator potential.

2 Theory

2.1 Jac

3 Method

The first step of solving eigenvalue problems numerically, is of course to set up the matrix. In both the case of solving the buckling beam problem and the quantum mechanical problem the matrix is a tridiagonal matrix. In the case of the buckling beam problem the matrix becomes very simple, the diagonal elements are all equal, and the non-diagonal elements are all equal. (referer til hvilke verdier som skal brukes for diag-elementer og nondiag-elementer, gitt i teori). We find the analytical eigenvalues by using armadillos functions for diagonalizing a matrix. These values are to be compared with values found using the Jacobi method.

The general expression for the new matrix elements are:

$$b_{ii} = a_{ii}, i \neq k, i \neq l$$

$$
\begin{aligned}
b_{ik} &= a_{ik}\cos\theta - a_{il}\sin\theta, i \neq k, i \neq l \\
b_{il} &= a_{il}\cos\theta + a_{ik}\sin\theta, i \neq k, i \neq l \\
b_{kk} &= a_{kk}\cos^2\theta - 2a_{kl}\cos\theta\sin\theta + a_{ll}\sin^2\theta \\
b_{ll} &= a_{ll}\cos^2\theta + 2a_{kl}\cos\theta\sin\theta + a_{kk}\sin^2\theta \\
b_{kl} &= (a_{kk} - a_{ll})\cos\theta\sin\theta + a_{kl}(\cos^2\theta - \sin^2\theta) \qquad (1)
\end{aligned}
$$

4 Implementation

5 Results

6 Discussion

7 Concluding remarks

References