Project 2 in FYS3150

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1 ABSTRACT

In this project we have coded a implementation of Jacobi's rotation algorithm, that finds an approximation to differential equations. We then then used this to model a harmonic oscillator problem in three dimensions, with one and two electrons.

2 INTRODUCTION

3 METHOD

3.a Mathematical basis

3.b Basic code, eller noe

3.c Testing the code

3.d Quantum dots in three dimensions, one electron

Now that we had a general algorithm we used it to model a electron that moves in a three-dimensional harmonic oscillator potential. In other words, we looked for the solution of the radial part of Schroedinger's equation for one electron, which reads

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{l(l+1)}{r^2}\right)R(r)+V(r)R(r)=ER(r). \tag{1}$$

This problem also has analytical solutions, so we can test how accurate our algorithm is.

(Some math-stuff).

The Schroedinger's equation then becomes

$$-\frac{d^2}{d\rho^2}u(\rho)+\rho^2u(\rho)=\lambda y(\rho). \tag{2}$$

Since we are working in radial coordinates we have $\rho \in [0,\infty)$. Since we can't represent infinity on a computer we have to find an aproximation, which we will come back to later. For now we define $\rho_{min}=0$ and ρ_{max} to represent the minimum and maximum values of ρ.

Function 2 is an differential equation that can be modeled similarly to (ting). If we have n mesh points we get a step length

$$h=\frac{\rho_{max}-\rho_{min}}{n}. \tag{3}$$

3.e Quantum dots in three dimensions, two electrons

4 RESULTS

5 CONCLUSIONS

6 APENDICES

7 REFERENCES