Report 2

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We are a bit behind schedule. This is an incomplete report. For the newest version of the report visit github.

1 Abstract

2 Introduction

The aim of this project is to create a program that finds eigenvalues with Jacobi's(Givens') method. We start off with studying the quantum mechanical problem of a particle in an infinite potential well, generating a general solution to find the eigenvalues of a matrix. Then moving on to two particles with Coulomb interactions.

3 Underlying theory

For electrons it is safe to assume a sentro symmetric potential, making it reasonable to use spherical coordinates. Here the angle dependent parts of the Schrödinger equation is independent of the position r. To model the electron further only the radial part of the SE is needed.

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}-\frac{l(l+1)}{r^2}\right)R(r)+V(r)R(r)=ER(r) \qquad r\in[0,\infty) \tag{1}$$

Here $V(r)=(1/2)m\omega^2r^2$ the middle term can be expressed as $m\omega^2=k$. The eigenvalues(E) are here the energy of the harmonic oscillator. The frequency ω of the system are given as:

$$E_{nl}=\hbar\omega\left(2n+l+\frac{3}{2}\right) \qquad n,l=0,1,2,3... \tag{2}$$

Here the variable l is the orbital momentum of the electron. To further simplify the expression a substitution of variables can be made.

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}-\frac{l(l+1)}{r^2}\right)R(r)+V(r)R(r)=ER(r)$$
$$R(r)=\frac{1}{r}u(r) \qquad u(0)=u(\infty)=0$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2u(r)}{\partial r^2}+\left(V(r)+\frac{l(l+1)}{r^2}\frac{hbar^2}{2m}\right)u(r)=Eu(r)$$

3.1 Generalization

To beam this specific example into a more general one dimensionless variables were introduced. $\rho = (1/\alpha)r$ is introduced with α having the dimension length. l is fixed to zero.

$$-\frac{\hbar^2}{2m\alpha^2}\frac{\partial^2 u(\rho)}{\partial\rho^2} + V(\rho)u(\rho) = Eu(\rho)$$

The potential is now defined to $V(\rho) = (1/2)k\alpha^2\rho^2$.

$$-\frac{\hbar^2}{2m\alpha^2}\frac{\partial^2 u(\rho)}{\partial\rho^2} + \frac{1}{2}k\alpha^2\rho^2 u(\rho) = Eu(\rho)$$
$$-\frac{\partial^2 u(\rho)}{\partial\rho^2} + \frac{m}{\hbar^2}k\alpha^4\rho^2 u(\rho) = \frac{2m\alpha^2}{\hbar^2}Eu(\rho)$$

To remove the units in the potential one can set $\alpha = \sqrt[4]{\frac{\hbar^2}{mk}}$, and the variables on the right hand side can be defined as $\lambda = \frac{2m\alpha^2}{\hbar^2} = E$

$$-\frac{\partial^2 u(\rho)}{\partial\rho^2} + \rho^2 u(\rho) = \lambda u(\rho) \tag{3}$$

This is now reduced to a general second derivative discrete function and can be expressed as:

$$\frac{\partial^2 u(\rho)}{\partial\rho^2} = \frac{u(\rho+h) - 2u(\rho) + u(\rho-h)}{h^2} + O(h^2) \tag{4}$$

Here h is the step length. The limits of the new variable ρ also needs to be defined. The lower limit, $r_{\min} = 0 \to \rho = 0$ is fine, but the upper limit causes trouble. Here $r_{\max} = \infty \to \rho = \infty$. This is not possible to represent on a computer. Since the function now has a discrete approximation a discrete value can also be given for the upper limit. $\rho = \rho_{\max}$. The step length will now be defined from the total amount of steps in the approximation.

$$h = \frac{\rho_{\max} - \rho_{\min}}{N}$$

Indexing the steps after the number of steps taken will further be beneficial.

$$\rho_0 \cdots \rho_i \cdots \rho_N \qquad i = 0, 1, 2....N$$
$$\rho_i = \rho_0 + hi$$

Rewriting

$$\frac{\partial^2 u(\rho)}{\partial\rho^2} = \frac{u(\rho+h) - 2u(\rho) + u(\rho-h)}{h^2} + O(h^2) \tag{5}$$

Applying the step-wise ρ_i to the general result 3, inserting 4 gives:

$$-\frac{u(\rho_i + h) - 2u(\rho_i) + u(\rho_i - h)}{h^2} + \rho_i^2 u(\rho_i) = \lambda u(\rho_i)$$

A short hand notation of this would be to bring the variable the function u works on into the subscript, $u(\rho_i) = u_i$.

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + V_i^2 u_i = \lambda u_i \tag{6}$$

Systematizing this result into a matrix were a column represents u_i will yield the following:

$$\begin{bmatrix} \frac{2}{h^2} + V_1 & -\frac{1}{h^2} & 0 & 0 & \dots & 0 & 0 \\ -\frac{1}{h^2} & \frac{2}{h^2} + V_2 & -\frac{1}{h^2} & 0 & \dots & 0 & 0 \\ 0 & -\frac{1}{h^2} & \frac{2}{h^2} + V_3 & -\frac{1}{h^2} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & -\frac{1}{h^2} & \frac{2}{h^2} + V_{N-2} & -\frac{1}{h^2} \\ 0 & \dots & \dots & \dots & \dots & -\frac{1}{h^2} & \frac{2}{h^2} + V_{N-1} \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ \dots \\ \dots \\ \dots \\ u_N \end{bmatrix} = \lambda \begin{bmatrix} u_0 \\ u_1 \\ \dots \\ \dots \\ \dots \\ u_N \end{bmatrix} \tag{7}$$

Note here that the end and start columns have been removed due to them being known from the boundary conditions. From the matrix one can define a better short hand notation for the values:

The diagonal matrix elements:

$$d_i = \frac{2}{h^2} + V_i,$$

The non-diagonal matrix elements:

$$e_i = -\frac{1}{h^2}.$$

4 Method

5 Result

6 Discussion

7 Conclusion