FYS4150 Project 2:
Schrödinger's equation for two electrons in a 3-dimensional harmonic oscillator well

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Abstract

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1 Introduction

The aim of this project is to solve Schrödinger's equation for two electrons in a three-dimensional harmonic oscillator well with and without a repulsive Coulomb interaction. We are first interested in the solution of the radial part of Schrödinger's equation for *one* electron. This equation reads

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

In our case $V(r)$ is the harmonic oscillator potential $(1/2)kr^2$ with $k = m\omega^2$ and E is the energy of the harmonic oscillator in three dimensions. The quantum number l is the orbital momentum of the electron. The oscillator frequency is ω and the energies are

$$E_{nl} = \hbar\omega\left(2n + l + \frac{3}{2}\right), \quad (2)$$

with $n = 0, 1, 2, \ldots$ and $l = 0, 1, 2, \ldots$. In this project we use $l = 0$.

We will solve Eq. (1) by reformulating it in a discretized form as an eigenvalue equation to be solved with Jacobi's method.

After some substitutions and introducing the dimensionless variable $\rho = (1/\alpha)r$ where α is of dimension length, we can rewrite Eq. (1) as

$$-\frac{d^2}{d\rho^2}u(\rho) + \rho^2 u(\rho) = \lambda u(\rho). \quad (3)$$

This is the first equation to solve numerically. In three dimensions the eigenvalues for $l = 0$ are $\lambda_0 = 3, \lambda_1 = 7, \lambda_2 = 11, \ldots$.

We use the by now standard expression for the second derivative of a function u

$$u'' = \frac{u(\rho + h) - 2u(\rho) + u(\rho - h)}{h^2} + O(h^2), \quad (4)$$

where h is our step length. For a given number of steps n_{step}, the step length is defined as

$$h = \frac{\rho_{\max} - \rho_{\min}}{n_{\text{step}}}. \quad (5)$$

Next we define minimum and maximum values for the variable ρ, $\rho_{\min} = 0$ and $\rho_{\max}$, respectively. Define an arbitrary value of ρ as

$$\rho_i = \rho_{\min} + ih \qquad i = 0, 1, 2, \ldots, n_{\text{step}}. \quad (6)$$

Now we can write the Schrödinger equation in a compact way

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \rho_i^2 u_i = -\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + V_i u_i = \lambda u_i, \quad (7)$$

where $V_i = \rho_i^2$ is the harmonic oscillator potential.

Define first the diagonal matrix element

$$d_i = \frac{2}{h^2} + V_i, \quad (8)$$

and the non-diagonal matrix element (which is a mere constant, and are all equal)

$$e_i = -\frac{1}{h^2}. \quad (9)$$

With these definitions the Schrödinger equation takes the following form

$$d_i u_i + e_{i-1}u_{i-1} + e_{i+1}u_{i+1} = \lambda u_i, \quad (10)$$

where u_i is unknown. We can write the latter equation as a matrix eigenvalue problem

$$
\begin{pmatrix}
d_1 & e_1 & 0 & 0 & \ldots & 0 & 0 \\
e_1 & d_2 & e_2 & 0 & \ldots & 0 & 0 \\
0 & e_2 & d_3 & e_3 & 0 & \ldots & 0 \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 & \ldots & \ldots & \ldots & \ldots & d_{n_{\text{step}}-2} & e_{n_{\text{step}}-1} \\
0 & \ldots & \ldots & \ldots & \ldots & e_{n_{\text{step}}-1} & d_{n_{\text{step}}-1}
\end{pmatrix}
\begin{pmatrix}
u_1 \\ u_2 \\ \ldots \\ \ldots \\ \ldots \\ u_{n_{\text{step}}-1}
\end{pmatrix}
= \lambda
\begin{pmatrix}
u_1 \\ u_2 \\ \ldots \\ \ldots \\ \ldots \\ u_{n_{\text{step}}-1}
\end{pmatrix}
\tag{11}
$$

Secondly, we will consider the Schrödinger equation for *two* electrons by studying two electrons in a harmonic oscillator well which also interact via a repulsive Coulomb interaction.

We start by writing the single-electron equation as

$$
-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r) + \frac{1}{2}kr^2u(r) = E^{(1)}u(r),
\tag{12}
$$

where $E^{(1)}$ stands for the energy with one electron only. For two electrons with *no* repulsive Coulomb interaction, we have the following Schrödinger equation:

$$
\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr_1^2} - \frac{\hbar^2}{2m}\frac{d^2}{dr_2^2} + \frac{1}{2}kr_1^2 + \frac{1}{2}kr_2^2\right)u(r_1, r_2) = E^{(2)}u(r_1, r_2).
\tag{13}
$$

After a series of substitutions, this can be written as

$$
-\frac{d^2}{d\rho^2}\psi(\rho) + \omega_r^2\rho^2\psi(\rho) + \frac{1}{\rho} = \lambda\psi(\rho)
\tag{14}
$$

2 Methods

2.1 Jacobi's method

In this project we will use Jacobi's method to find the eigenvalues, which consists of doing a number of similarity transformations

$$
\mathbf{S}^T\mathbf{A}\mathbf{S} = \mathbf{B}
\tag{15}
$$

where $\mathbf{A}$ is the matrix in our given problem, and $\mathbf{S}$ is an $(n \times n)$ orthogonal transformation matrix

$$
\mathbf{S} =
\begin{pmatrix}
1 & 0 & \ldots & 0 & 0 & \ldots & 0 & 0 \\
0 & 1 & \ldots & 0 & 0 & \ldots & 0 & 0 \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & 0 & \ldots \\
0 & 0 & \ldots & \cos\theta & 0 & \ldots & 0 & \sin\theta \\
0 & 0 & \ldots & 0 & 1 & \ldots & 0 & 0
\end{pmatrix}
\tag{16}
$$

(MATRIX NOT FINISHED)

3 Results

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4 Conclusions

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5 List of codes

The codes developed for this project are:

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