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

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

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

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

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

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

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

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

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

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

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

2 Methods

2.1 Jacobi's method

3 Results

4 Conclusions

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5 List of codes

The codes developed for this project are:

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