Project 2

FYS4150 Computational Physics

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Abstract

1 Introduction

The purpose of this project is to develop a program for solving eigenvalue problems by using Jacobi's algorithm.

2 The Schrödinger equation

(This section follows very closely the theoretical introduction given project description, but for completeness sake I thought it would be nice to also include it in the report.)

2.1 One-particle case

We start by considering the radial part of the Schrödinger equation (SE) for one electron, which is given as

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

where (in our case) $V(r)$ is the harmonic oscillator (HO) potential

$$V(r)=\frac{1}{2}kr^2,$$

where $k=m\omega^2$. E is then the energy of the three dimensional HO, ω is the oscillator frequency, and these quantities are related by

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

where $n=0,1,2,\ldots$ and $l=0,1,2,\ldots$. Throughout this project only cases with $l=0$ will be considered.

By making the substitution $R(r)=(1/r)u(r)$ and introducing the dimensionless variable $\rho=(1/\alpha)r$ eq. (1) can be simplified to

$$-\frac{\hbar^2}{2m\alpha^2}\frac{d^2}{d\rho^2}u(\rho)+\frac{k}{2}\alpha^2\rho^2u(\rho)=Eu(\rho),$$

with boundary conditions $u(0)=u(\infty)=0$. Further we can multiply the equation by $2m\alpha^2/\hbar^2$, and fix α so that

$$\frac{mk}{\hbar^2}\alpha^4=1.$$

If we also define

$$\lambda=\frac{2m\alpha^2}{\hbar^2}E$$

we end up with the eigenvalue equation

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

We must of course make a discrete approximation to the equation in order to solve the problem numerically. However, before moving on to that we should have a quick look at the changes that are introduced by adding a second electron to the problem.

2.2 Two-particle case

The radial SE for two electrons in an HO potential without any interactions is given by

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr_1^2} - \frac{\hbar^2}{2m}\frac{d^2}{dr_2^2} + \frac{1}{2}kr_1^2 + \frac{1}{2}kr_2^2\right)u(r_1, r_2) = E^{(2)}u(r_1, r_2), \tag{3}$$

where $E^{(2)}$ is the two-electron energy. The solution to this equation is just the product of the wave functions for each electron. However, when we introduce the Coulomb interaction (which depends on the distance r between the electrons) eq. (3) is not very useful. For that reason we would like to introduce a new set of coordinates, namely the relative distance between the electrons,

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2,$$

and the centre-of-mass coordinate for the system,

$$\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2).$$

The SE (still without interactions) can then be written as

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} - \frac{\hbar^2}{4m}\frac{d^2}{dR^2} + \frac{1}{4}kr^2 + kR^2\right)u(r, R) = E^{(2)}u(r, R),$$

where $r = |\mathbf{r}_1 - \mathbf{r}_2|$ and $R = \frac{1}{2}|\mathbf{r}_1 + \mathbf{r}_2|$. We then assume that the wave function is separable, so that $u(r, R) = \psi(r)\phi(R)$, and that the total energy is given by the sum of relative energy, E_r, and centre-of-mass energy, E_R, i.e.

$$E^{(2)} = E_r + E_R.$$

We can then add the term for the Coulomb interaction, which is given by

$$V(r) = \frac{\beta e^2}{r},$$

where $\beta e^2 = 1.44$ eVnm, and the r-dependent part of the SE becomes

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \frac{1}{4}kr^2 + \frac{\beta e^2}{r}\right)\psi(r) = E_r\psi(r).$$

As we did for the one-electron SE we now introduce the dimensionless variable $\rho = r/\alpha$, and scale the equation appropriately. After a few steps of manipulation we arrive to

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \omega_r^2\rho^2\psi(\rho) + \frac{1}{\rho} = \lambda\psi(\rho), \tag{4}$$

where

$$\omega_r^2 = \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4,$$

with α fixed so that

$$\frac{m\alpha\beta e^2}{\hbar^2} = 1,$$

and λ is defined as

$$\lambda = \frac{m\alpha^2}{\hbar^2}E.$$

It is noteworthy that the only differences between equations (2) and (4) is the factor ω_r^2 in the HO potential term, and the Coulomb repulsion term. This means that it is quite easy to make the transition between these cases when writing the code, which is in fact the main point of doing the scaling.

2.3 Discrete Schrödinger equation

As mentioned previously we must make a discrete approximation to the SE, and when doing so we will jump back to the one-electron problem, i.e. eq. (2).

The second derivative is approximated (up to $O(h^2)$) by

$$u'' \approx \frac{u(\rho+h) - 2u(\rho) + u(\rho-h)}{h^2},$$

where h is the step length. The minimum value of ρ is $\rho_{min} = \rho_0 = 0$, while the maximum value is in principle infinity. However, infinity is not a very practical "value" to work with, especially in a numerical context, which means that we must choose an appropriate maximum value $\rho_{max} = \rho_N$. The step length h is then defined as

$$h = \frac{\rho_N - \rho_0}{N},$$

where N is the number of mesh points we consider, and ρ is given as

$$\rho_i = \rho_0 + ih,$$

with $i = 1, 2, \ldots, N$. By using the short-hand notation $u(\rho_i + h) = u_{i+1}$, we can write the SE as

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + V_i u_i = \lambda u_i, \tag{5}$$

where $V_i = \rho_i^2$ is the HO potential. This is now an eigenvalue problem which can be compactly written as $\mathbf{Au} = \lambda\mathbf{u}$, where $\mathbf{A}$ is a matrix with diagonal elements

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

and non-diagonal elements

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

If we instead want to consider the two-electron case with Coulomb interaction we simply change the potential V_i from ρ_i^2 to $\omega_r^2\rho_i^2 + 1/\rho_i$.

3 The Jacobi algorithm

3.1 Implementation of the Jacobi algorithm

4 Results

5 Summary and conclusions