FYS3150 - Project 2

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Abstract

We investigate a numerical solution to Schroedinger's equation for two electrons confined in a three-dimensional harmonic oscillator well. We present a solution to the case where we disregard the interaction between the electrons, and a solution where we include a repulsive (Coloumb) interaction between the electrons.

Contents

1 Introduction

The study of electrons confined in a potential trap is a highly active research field today **INSERT SOME REFERENCES HERE**, due to its potential applicability in solid-state physics. Some proposed applications for these systems include semi-conductors and quantum gates for future quantum computers, as well as nano-medical applications.

We investigate Schroedinger's equation for two non-interacting electrons confined in a three-dimensional potential well, and reformulate it as an Eigenvalue problem. We then solve this problem by use of Jacobi's method for finding eigenvalues and eigenvectors. Once we have developed this general method, it is straightforward to implement the potential for the interacting electrons.

2 Theoretical model

2.1 Introducing the relevant Schroedinger equation

A three-dimensional potential well is described by the harmonic oscillator potential:

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

Here r is the distance from the origin, and k is a constant describing the steepness of the well. Note how this potential is radially symmetric. This means that we can ignore the angular parts of the Schroedinger's equation, leaving us with the radial equation:

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

Here E is the energy of the harmonic oscillator, and l are orbital momentum numbers[1]. Substituting $R(r) = \frac{u(r)}{r}$ as done **INSERT REFERENCE HERE**, we obtain:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r) + \left(V(r) + \frac{l(l+1)}{r^2}\frac{\hbar^2}{2m}\right)u(r) = Eu(r) \tag{3}$$

[1] Our background in quantum mechanics being nonexistent, we assume this sentence to be meaningful.

From this transformation, it also follows that the boundary conditions are necessarily $u(0) = u(\infty) = 0$.

2.2 Introducing the potentials

We will consider the case of two electrons. Note that this transforms the above equation to a system of two differential equations. The system will be coupled if the electrons interact with each other and decoupled if they do not. The decoupled case is identical to the case of a single electron, because the electrons are identical. The interacting case is slightly more complicated, but it can be simplified by introducing the center of mass (COM) coordinate, R, as:

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

Where $\vec{r}_1$ and $\vec{r}_2$ are the position vectors of the electrons. We can then employ a standard separation of variables approach, inserting an Ansatz of the form

$$u(r, R) = \psi(r)\phi(R)$$

Note that we are only interested in the difference between the position of the electrons (the COM coordinate should given an equation similar to the non-interacting case). Thus we can consider only the r equation.

We will be investigating two different potentials. We will begin by simply imposing a harmonic oscillator (HO) potential, of the form:

$$V(r)_{HO} = \frac{1}{2}kr^2 \tag{4}$$

I.e, we confine the electrons in a parabolic potential.We will subsequently consider the repulsive force between the electrons. This will be modelled by a simple Coloumb potential, of the form:

$$V(r)_{Coloumb} = \frac{1}{4\pi\epsilon_0}\frac{q}{r} \tag{5}$$

Where q is the charge of an electron and r is the distance between the electrons. The total potential in this case will be a linear superposition of equation 4 and equation 5.

We have now clarified the mathematical framework. It is convenient, however, to scale the presented equations. The details of this scaling can be found **here**. A slightly different scaling is needed for the interacting case than for the non-interacting case. The potential, in terms of a dimensionless parameter ρ, for the non-interacting case simply becomes:

$$V(\rho)_{HO} = \rho^2$$

For the interacting case, the potential becomes.

$$V(\rho)_{tot} = V(\rho)_{HO} + V(\rho)_{coloumb} = \omega_r^2\rho^2 + 1/\rho$$

Where ω_r is a characteristic frequency defined **HERE**. This parameter specifies the strength of the harmonic oscillator potential.

2.3 Reformulating the equation as an Eigenvalue problem

After the reformulation from the previous section, Schroedinger's equation for two electrons can now be written as:

$$-\frac{d^2}{d\rho^2}u(\rho) + V(\rho)u(\rho) = \lambda u(\rho) \tag{6}$$

Where ρ is a dimensionless quantity describing a characteristic length and λ are the (sought-after) eigenvalues of the system. V is the chosen potential. To reformulate this as an Eigenvalue problem, we discretize the second derivative in the equation. This implies that we write the continuous function $u(\rho)$ as a function at discrete points, $u(\rho_i) = u_i$, with $i = 0, 1, ..., N$. We can then expand the second derivative in terms of Taylor polynomials to get an iterative scheme for solving the differential equation. The detailed procedure can be found **HERE**, with the final result:

$$d_i u_i + e_{i-1} u_{i-1} + e_{i+1} u_{i+1} = \lambda u_i \tag{7}$$

Where $d_i = 2/h^2 + V_i$ and $e_i = -1/h^2$, with h being the step length (distance between ρ_i and ρ_{i+1}). Note how every e is the same, i.e. we can define $e_i = e$. This can now be reformulated as an eigenvalue problem with a tridiagonal matrix, $\mathbf{A}$ that is:

$$\mathbf{A}\mathbf{u} = \lambda \mathbf{u} \tag{8}$$

The matrix $\mathbf{A}$ is found by inserting the u and e from above, giving:

$$\mathbf{A} = \begin{bmatrix} d_0 & e & 0 & 0 & \dots & 0 & 0 \\ e & d_1 & e & 0 & \dots & 0 & 0 \\ 0 & e & d_2 & e & 0 \dots & 0 & \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & e & d_{N-1} & e \\ 0 & \dots & \dots & \dots & \dots & e & d_N \end{bmatrix}$$

2.4 Implementing the boundary conditions

As shown in section 2.1, the problem under considerations has Dirichlet-type boundary conditions of the form $u(0) = u(\infty) = 0$. Inserting these conditions into equation 7 gives:

$$(d_1 - \lambda)u_1 + eu_2 = 0$$

Note, however, that u_0 and u_N are known, and thus we can remove those rows and columns from the matrix.

2.5 Jacobi's algorithm for solving an eigenvalue problem

Equation 8 can be solved via a general algorithm known as Jacobi's method. Details of this method can be found **HERE**, but the general idea is rather straightforward. The method hinges on the fact that it is extremely easy to find the Eigenvalues of a diagonal matrix, $\mathbf{D}$ - they are simply the diagonal elements. We employ a series of orthogonal transformations , $\mathbf{S}_i$, as:

$$\mathbf{S}_n^T \mathbf{S}_{n-1}^T ... \mathbf{S}_1^T \mathbf{A} \mathbf{S}_1 \mathbf{S}_2 ... \mathbf{S}_n$$

where the goal is to arrive at a matrix that is (almost) diagonal - that is, all off-diagonal elements are smaller than some threshold value, ϵ. We chose the matrix $\mathbf{S}$ to be a rotation matrix, which zeros out one element at a time. This leads to a quadratic equation in the tan of the rotation angle, which can be solved for the corresponding sines and cosines. The detailed explanation can be found **here**, but the final quadratic equation is:

$$t = -\tau \pm \sqrt{1 + \tau^2} \tag{9}$$

Where t is the tan of the rotation angle, and τ is a parameter depending on the matrix element we wish to zero out. Note that, because this is a rotational matrix and $\tan(x)$ is symmetric, we can always choose the smaller of the two solutions (corresponding to the smaller angle). Thus, if τ is negative, we can choose the positive solution, and vice versa.

Two important points must be noted from the more detailed explanation. First of all, we must always choose the largest non-zero off-diagonal matrix element to zero out. This ensure monotonous behavior, so that the elements which are zero at one point stay zeroed out. Secondly, whilst equation 9 looks neat mathematically, one should rewrite it slightly in the numeric implementation. If $\tau >> 1$ then $\sqrt{1+\tau^2} \approx |\tau|$. Subtracting two almost equal numbers numerically can lead to a loss of precision due to round-off errors. Therefore, one should rewrite the equation slightly. For $\tau \geq 0$:

$$-\tau + \sqrt{1+\tau^2} = \frac{(-\tau + \sqrt{1+\tau^2})(-\tau - \sqrt{1+\tau^2})}{-\tau - \sqrt{1+\tau^2}} = \frac{\tau^2 - 1 - \tau^2}{-\tau - \sqrt{1+\tau^2}} = \frac{1}{\tau + \sqrt{1+\tau^2}} \tag{10}$$

For $\tau < 0$:

$$-\tau - \sqrt{1+\tau^2} = \frac{(-\tau - \sqrt{1+\tau^2})(-\tau + \sqrt{1+\tau^2})}{-\tau + \sqrt{1+\tau^2}} = \frac{\tau^2 - 1 - \tau^2}{-\tau + \sqrt{1+\tau^2}} = \frac{-1}{-\tau + \sqrt{1+\tau^2}} \tag{11}$$

Which are the equations we implemented in our algorithm.

2.6 Investigating the properties of orthogonal transfomrations

We will here briefly investigate some properties of orthogonal transforms, to arrive at possible unit tests to implement in our programs. We will show that this transformation preserves the dot product and orthogonality. Thus let $\mathbf{v}_i$ and $\mathbf{v}_j$ be two arbitrary vectors. Consider an orthogonal transformation matrix, $\mathbf{U}$, that is $\mathbf{U}^T = \mathbf{U}^{-1}$. Define $\mathbf{w}_i = \mathbf{U}\mathbf{v}_i$ and $\mathbf{w}_j = \mathbf{U}\mathbf{v}_j$. Consider:

$$\mathbf{w}_i \cdot \mathbf{w}_j = (\mathbf{U}\mathbf{v}_i)^T (\mathbf{U}\mathbf{v}_j)$$

Where the last equality follows from the definition of the inner product. Using the properties of the transpose, the first parenthesis can be expanded as:

$$(\mathbf{U}\mathbf{v}_i)^T = \mathbf{v}_i^T \mathbf{U}^T$$

Multiplying this out gives:

$$\mathbf{w}_i \cdot \mathbf{w}_j = \mathbf{v}_i^T \mathbf{U}^T \mathbf{U}\mathbf{v}_j = \mathbf{v}_i^T \mathbf{I}\mathbf{v}_j = \mathbf{v}_i \cdot \mathbf{v}_j$$

This shows immediately that the orthogonal transformation preserves the dot product. It also shows, however,that it prerves orthogonality. To see this, assume therefore that we have a basis of orthonormal vectors, $\mathcal{B} = \{\mathbf{v}_i\}$, i.e. that $\mathbf{v}_i \cdot \mathbf{v}_j = \delta_{ij}$. Inserting this into the last expression gives:

$$\mathbf{w}_i \cdot \mathbf{w}_j = \delta_{ij}$$

Which shows that orthogonal transformations also preserve vector orthogonality.