FYS3150 - Project 2

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I. INTRODUCTION

The harmonic oscillator (HO) potential appears in many areas within quantum physics. This is because many potentials can be approximated, at least in some intervals, with a HO potential. The most famous example of this might be the model for a hydrogen atom, where the electron is bound to the proton by a HO potential. That is why, in this report, we are going to study both one and multiple electrons in a HO potential. We are also going to account for electrical forces between the particles.

II. THEORY

A. Unitary transformation

The transformed of a unitary matrix (U) is its inverse.

$$U^T = U^{-1}$$

From this we can prove that a unitary transformation preserves the orthonormality of vectors. Consider the set of orthonormal vectors $\{\mathbf{v}_i\}_i$ and the unitary transformation $\{U\mathbf{v}_i\}_i = \{\mathbf{w}_i\}_i$.

$$\begin{aligned}\mathbf{w}_i^T\mathbf{w}_j &= (U\mathbf{v}_i)^T U\mathbf{v}_j \\ &= \mathbf{v}_i^T U^T U\mathbf{v}_j = \mathbf{v}_i^T\mathbf{v}_j \\ &= \delta_{i,j}\end{aligned}$$

We notice that orthonormality is perserved.

B. Jacobi's rotation algorithm

Jacobi's rotation algorithm uses unitary transformations to diagonalize a matrix. A detailed description of the algorithm can be found here [1], however we will describe it briefly. In order to diagonalize a given matrix A, as mentioned over, we perform a series of unitary transformations.

$$B = U_n^T U_{n-1}^T ... U_0^T A U_0 ... U_{n-1} U_n$$

Here U_i are the unitary matrices and B the resulting diagonal matrix. An example of how U_i can look is given under.

$$\begin{bmatrix} 1 & 0 & ... & 0 & 0 & ... & 0 & 0 \\ 0 & 1 & ... & 0 & 0 & ... & 0 & 0 \\ ... & ... & ... & ... & ... & ... & 0 & ... \\ 0 & 0 & ... & \cos\theta & 0 & ... & 0 & \sin\theta \\ 0 & 0 & ... & 0 & 1 & ... & 0 & 0 \\ ... & ... & ... & ... & ... & ... & 1 & ... \\ 0 & 0 & ... & -\sin\theta & 0 & ... & 0 & \cos\theta \end{bmatrix}$$

The geometric interpretation is that U_i performs a rotation on T in order to zero out non-diagonal elements. It turns out that the fastest way to do this, is to zero out the largest non-diagonal matrix-element. First We define:

$$\cot(\theta) = \tau = \frac{a_{ll} - a_{kk}}{2a_{kl}},$$

Where a_{kl} is the largest non-diagonal element in A. Now to shorten notation we use $\tan(\theta) = t = s/c$, where $s = \sin(\theta) \wedge c = \cos(\theta)$. By defining θ such that a_{kl} becomes zero we get the quadratic equation

$$t^2 + 2\tau t - 1 = 0 \implies t = -\tau \pm \sqrt{1+\tau^2},$$

and can also obtain c and s

$$c = \frac{1}{1+t^2} \wedge s = tc.$$

The actual transformation is defined by the equations

$$\begin{aligned} b_{ik} &= a_{ik}c - a_{il}s, i \neq k, i \neq l \\ b_{il} &= a_{il}c + a_{ik}s, i \neq k, i \neq l \\ b_{kk} &= a_{kk}c^2 - 2a_{kl}cs + a_{ll}s^2 \\ b_{ll} &= a_{ll}c^2 + 2a_{kl}cs + a_{kk}s^2 \\ b_{kl} &= (a_{kk} - a_{ll})cs + a_{kl}(c^2 - s^2) \end{aligned}$$

Where b_{ij} are elements in B, again see [1] for a more detailed description of the algorithm.

C. Electrons in a harmonic oscillator potential

It turns out that if you try to solve Schrodinger's equation you end up with a eigenvalue problem. We will derive the math here, but everything is taken from here [2]. First we consider the Schrodinger's equation for one electron, we then, because of spherical symmetry, only need to look at the radial part.

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

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Where $R(r)$ is the radial wave equation, $V(r)$ the potential, l orbital momentum and r distance from the origin. Now because we only have one electron we end up with the HO potential $V(r) = (1/2)kr^2$. Substituting $R(r) = (1/r)u(r)$ and $\rho = (1/\alpha)r$ (where α is a constant with dimension length) we obtain

$$-\frac{\hbar^2}{2m\alpha^2}\frac{d^2}{d\rho^2}u(\rho)+\left(V(\rho)+\frac{l(l+1)}{\rho^2}\frac{\hbar^2}{2m\alpha^2}\right)u(\rho)=Eu(\rho).$$

Setting the orbital momentum $l = 0$, inserting $V(\rho) = (1/2)k\alpha^2\rho^2$ and defining

$$\alpha \equiv \left(\frac{\hbar^2}{mk}\right)^{1/4} \wedge \lambda \equiv \frac{2m\alpha^2}{\hbar}E$$

Schrodinger's equation can then be described by the simple equation (2).

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

Now we can expand our model to two particles with Coulomb potential between them. First introducing the relative position $\mathbf{r}$ and center-of-mass coordinate $\mathbf{R}$

$$\mathbf{r} = \mathbf{r_1} - \mathbf{r_2} \wedge \mathbf{R} \ = \frac{1}{2(\mathbf{r_1}+\mathbf{r_2})}.$$

Where $\mathbf{r_1}$ and $\mathbf{r_2}$ are the particles positions.Then the radial Schrodinger's becomes

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

$E^{(2)}$ denotes the fact that we are looking at the total energy of two particles. From an ansatz for the wave equation, we can perform separation of variable on r and R.

$$u(r,R) = \psi(r)\phi(R) \wedge E^{(2)} = E_r + E_R$$

Adding the Coulomb potential

$$\frac{\beta e^2}{r}$$

between the two electrons we get

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

Again introducing $\rho = r/\alpha$ and defining a few variables

$$\omega_r^2 \equiv \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4 \wedge \alpha \equiv \frac{\hbar^2}{m\beta e^2} \wedge \lambda \equiv \frac{m\alpha^2}{\hbar^2}E$$

We arrive at the Schrodinger's equation (3)

$$-\frac{d^2}{d\rho^2}\psi(\rho)+\omega_r^2\rho^2\psi(\rho)+\frac{1}{\rho}=\lambda\psi(\rho) \tag{3}$$

III. METHOD

IV. RESULTS

V. DISCUSSION

VI. CONCLUSION

[1] http://compphysics.github.io/ ComputationalPhysics/doc/pub/eigvalues/html/._eigvalues-bs011.html
[2] OPPGAVETEKST REF