Computational Physics Project 2

Curtis Rau and Benjamin Brophy
Michigan State University

In this project we saught to solve the Schrödinger Equation for two interacting electrons in a cylindrically symmetric harmonic oscillator potential. Potentials of this form are useful for simulating quantum dots. Of particular interest are the low lying energy levels for this system which only have known analytical solutions for a few special cases [1]. This paper gives an overview of the process of boiling down the Schrodinger equation to an ealily solvable one dimentional differential equation. Then the method of discretizing the differential equation, and translating it into a matrix equation is discussed. The Jacobi Method is introduced as the way in which the eigenvalues were obtained. The Householder Algorithm was used to check the results from Jacobi's Method and both methods were in excellent agreement.

I. INTRODUCTION

In this project we aim to solve Schrödinger's equation for two electrons in a three dimensional harmonic oscillator well with and without a repulsive Coulomb interaction, assuming that the move in a three dimensional harmonic oscillator potential. Here we have the Schrödinger for two electrons at r_1 and r_2 in such a potential

$$[-\frac{\hbar^2}{2m}\left(\nabla_1^2+\nabla_2^2\right)+\frac{1}{2}m\omega^2\left(r_1^2+r_2^2\right) +\frac{ke^2}{|r_1^2-r_2^2|}]\psi(r_1,r_2)=E\psi(r_1,r_2) \tag{1}$$

The Schrödinger equation can be transformed to the radial equation in center of mass frame, where r represents the distance between electrons, and R is the position of the center of mass.

$$[\left(-\frac{\hbar^2}{m}\frac{1}{r^2}\partial_r r^2\partial_r+\frac{1}{4}m\omega^2r^2+\frac{ke^2}{r}\right) +\left(-\frac{\hbar^2}{4m}\frac{1}{R^2}\partial_R R^2\partial_R+m\omega^2R^2+\frac{\hbar l(l+1)}{R^2}\right)] \psi(r)\theta(R)=(E_r+E_R)\psi(r)\theta(R) \tag{2}$$

We are only interested in the radial solution

$$\left(-\frac{\hbar^2}{m}\frac{1}{r^2}\partial_r r^2\partial_r+\frac{1}{4}m\omega^2r^2+\frac{ke^2}{r}\right)\psi(r)=E_r\psi(r) \tag{3}$$

We can make the equation dimensionless which gives

$$\left(-\partial_\rho^2+\rho^2+\frac{\beta}{\rho}\right)u(\rho)=\lambda u(\rho)\left(-\partial_\rho^2+V(\rho)\right)u(\rho)=\lambda u(\rho) \tag{4}$$

II. METHODS

We discretize the equation as follows, where b and a are the end points of our model using N internal points. (There are N+2 total including end points)

$$\begin{aligned} u(\rho)\rightarrow u(\rho_i)=u_i \\ \rho\rightarrow\rho_i=\rho_0+ih \\ h=\frac{b-a}{n+1} \\ a=0 \end{aligned} \tag{5}$$

And use the following expression as an approximation of the second derivative:

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

We can approximate the Schrödinger equation as

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

In terms of matrices, we have

$$\begin{pmatrix} \frac{2}{h^2}+V_1 & -\frac{1}{h^2} & & 0 \\ -\frac{1}{h^2} & \frac{2}{h^2}+V_2 & -\frac{1}{h^2} & \\ & & \ddots & \\ & & & -\frac{1}{h^2} \\ 0 & & -\frac{1}{h^2} & \frac{2}{h^2}+V_{N-1} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \cdots \\ \\ u_N \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \\ \cdots \\ \\ u_N \end{pmatrix} \tag{6}$$

We will call the NxN matrix $\hat{A}$. We will perform a Jacobi rotation on this matrix, represented by multiplying both sides by S_{ij}^T, which as an identity matrix except with $c=cos\theta$ in positions i,i and j,j, $s=sin\theta$ at position i,j, and $-s$ at position j,i for some angle θ.

$$S_{ij}^T = \begin{pmatrix} 1 & & & & & & 0 \\ & \ddots & & & & & \\ & & c & \dots & s & & \\ & & \vdots & & \vdots & & \\ & & -s & \dots & c & & \\ & & & & & \ddots & \\ 0 & & & & & & 1 \end{pmatrix} \quad (7)$$

Note that:

- Eigenvalues unchanged under orthogonal transforms such as a Jacobi rotation.
- Eigenvectors change, but the length is preserved.
- Dot product between vectors is conserved

$$\hat{A}x = \lambda x \quad (8)$$
$$S^T Ax = \lambda S^T x \quad (9)$$
$$S^T AS(S^T x) = \lambda(S^T x) \quad (10)$$

The values in the new matrix $\hat{A}' = S_{ij}^T \hat{A}$ can be found with the following relations, where $s = sin\theta$ and $c = cos\theta$ for some θ:

$$\hat{A}'_{ii} = c^2\hat{A}_{ii} - 2sc\hat{A}_{ij} + s^2\hat{A}_{jj} \quad (11)$$
$$\hat{A}'_{jj} = s^2\hat{A}_{ii} + 2sc\hat{A}_{ij} + c^2\hat{A}_{jj} \quad (12)$$
$$\hat{A}'_{ij} = \hat{A}'_{ji} = (c^2 - s^2)\hat{A}_{ij} + sc(\hat{A}_{ii} - \hat{A}'_{jj}) \quad (13)$$
$$\hat{A}'_{ik} = \hat{A}'_{ki} = c\hat{A}_{ik} - s\hat{A}_{jk}, k \neq i, j \quad (14)$$
$$\hat{A}'_{jk} = \hat{A}'_{kj} = s\hat{A}_{ik} - c\hat{A}_{jk}, k \neq i, j \quad (15)$$
$$\hat{A}'_{kl} = \hat{A}_{kl}, k, l \neq i, \quad (16)$$

We performed a Jacobian eigenvalue algorithm on this matrix to find the approximate eigenvalues. If we minimize all of the off-diagonal elements with orthogonal transforms, which preserve eigenvalues, then the remaining diagonal gives us the approximate eigenvalues of the matrix. A Jacobi rotation is one such orthogonal transform.

In our method, we first identify the largest off-diagonal element $A_{i,j}$ to use as the "pivot" in the Jacobi Rotation. So, we find the angle of rotation such that $A_{i,j}$ becomes zero. We perform a Jacobi rotation of that angle on $\hat{A}$ and call the rotated matrix our new $\hat{A}$.

We repeat this process until either the largest off-diagonal element has absolute value less than a certain tolerance, 0.01, or until a maximum number of iterations is reached.

After many iterations, the off diagonal elements are minimized while the diagonals elements approach eigenvalues.

III. ANALYSIS

- for part B, using N = 200 and rhoMax = 5.0 gives the three lowest eigenvalues up to 3 decimal places.

A. Part B

IV. CONCLUSIONS

[1] M. Taut. Two electrons in an external oscillator potential: Particular analytic solutions of a coulomb correlation potential. *Physical Review A*, 48(5):3561–3566, November 1993.

Size of Matrix	Tolerance	Householder Time	Jacobi Time	Itterations of Jacobi Method	Jacobi E1	Householder E1
100	0.1	0.01	0.15	8684	3.00030	3.22937
”	0.01	”	0.20	10667	2.99924	”
”	0.001	”	0.21	12076	2.99923	”
”	0.0001	”	0.25	13200	”	”
200	0.1	0.1	2.5	36836	3.00228	2.99986
”	0.01	”	2.9	44012	2.99981	”
”	0.001	”	3.2	49387	”	”
”	0.0001	”	3.6	53888	”	”
300	0.1	0.38	12.2	85521	3.00024	3.00000
500		2.9				3.00003
750		9.7				3.00006
1000		54.6				2.99967

TABLE I: rhoMax = 5.0