PHY905 Project 2 - Jacobi Algorithm

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Background:
Purpose:
Method:
Results:
Conclusions:

I. INTRODUCTION

For a single electron in a harmonic oscillator potential, the radial Schrödinger equation is given by:

$$\frac{\hbar}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{\ell(\ell+1)}{r^2}\right)R_n(r) \\ +\frac{1}{2}m\omega^2r^2R_n(r)=E_{n\ell}R_n(r) \qquad (1)$$

where $R_n(r)$ are the radial wave functions, ω is the oscillator frequency, and $E_{n\ell}$ is the energy for the given quantum numbers:

$$E_{n\ell}=\hbar\omega\left(2n+\ell+\frac{3}{2}\right) \quad n,\ell=0,1,2... \qquad (2)$$

In this work we will focus on $\ell=0$. Then making the substitution $u_n(r)=rR_n(r)$ and $\rho=\alpha/r$ where $\alpha^4=\hbar^2/mk$ and $k=m\omega^2$ gives:

$$-\frac{d^2}{d\rho^2}u_n(\rho)+\rho^2u_n(\rho)=\frac{2m\alpha}{\hbar^2}E_nu_n(\rho). \qquad (3)$$

Simplifying further, we can introduce the variable λ such that:

$$-\frac{d^2}{d\rho^2}u_n(\rho)+\rho^2u_n(\rho)=\lambda u_n(\rho). \qquad (4)$$

This equation can be solved analytically to give the eigenvalues $\lambda_0=3$, $\lambda_0=7$, and $\lambda_2=11$.

If rather than one electron in the harmonic oscillator well there are two which are non-interacting, then Equation 1 becomes:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr_1^2}-\frac{\hbar^2}{2m}\frac{d^2}{dr_2^2}+\frac{1}{2}kr_1^2+\frac{1}{2}kr_2^2\right)u_n(r_1,r_2) \\ =E_n^{(2)}u_n(r_1,r_2) \qquad (5)$$

where $u_n(r_1,r_2)$ is a two-body wave function and $E_n^{(2)}$ is the two-electron energy. We introduce new coordinates, $\mathbf{r}$ and $\mathbf{R}$, defined by:

$$\mathbf{r}=\mathbf{r_1}-\mathbf{r_2} \qquad (6)$$

$$\mathbf{R}=\frac{1}{2}\left(\mathbf{r_1}+\mathbf{r_2}\right) \qquad (7)$$

where $\mathbf{r}$ is the relative coordinate and $\mathbf{R}$ is the relative center-of-mass coordinate. This simplifies Equation 5 to:

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2}-\frac{h^2}{4m}\frac{d^2}{dR^2}+\frac{1}{4}kr^2+kR^2\right)u_n(r,R) \\ =E_n^{(2)}u_n(r,R) \qquad (8)$$

and allows for the both the wave function and the energy to be written in terms of a relative wave function and energy, $\psi(r)$ and E_r, and a center-of-mass wave function and energy, $\phi(R)$ and E_R:

$$u(r,R)=\psi(r)\phi(R) \qquad (9)$$

$$E^{(2)}=E_r+E_R. \qquad (10)$$

This change of variables proves even more useful though when a repulsive Coulomb interaction is included as:

$$V(r_2,r_2)=\frac{\beta e^2}{|\mathbf{r}_1-\mathbf{r}_2|}=\frac{\beta e^2}{r} \qquad (11)$$

where $\beta e^2=1.44$ eVnm. As this potential only depends on the relative coordinate, we can look exclusively at the Schrödinger equation for the relative wave function:

$$\left(-\frac{h^2}{m}\frac{d^2}{dr^2}+\frac{1}{4}kr^2+\frac{\beta e^2}{r}\right)\psi(r)=E_r\psi(r). \qquad (12)$$

Again we can make the substitution $\rho=r/\alpha$ where now $\alpha=\hbar^2/m\beta e^2$. In addition, we introduce the frequency $\omega_r=mk\alpha^4/4\hbar^2$, which reflects the strength of the oscillator potential, and the variable $\lambda=m\alpha^2E_r/\hbar^2$. Equation 12 then becomes:

$$-\frac{d^2}{d\rho^2}\psi(\rho)+w_r^2\rho^2\psi(\rho)+\frac{1}{\rho}=\lambda\psi(\rho). \qquad (13)$$

This equation has been solved analytically for some values of ω_r in [1]. Of specific interest in this work is the case $\omega_r=0.05$, where the ground state eigenvalue is given by $\lambda=0.35$.

In this work we implement the Jacobi algorithm to solve the eigenvalue problems described above and study the performance characteristics and numerical accuracy for different grid and step sizes. In addition, we investigate the influence of the frequency w_r on the shape of the wave functions in the interacting case. In Section II, the implementation of the algorithm is described. In Section III the performance and accuracy of the code are analyzed. Finally, in Section IV we give a summary and our conclusions.

II. METHODS

We first start by discretizing the functions in Equations 4 and 13 and approximating the derivatives as:

$$u'' = \frac{u(\rho+h) - 2u(\rho) + u(\rho-h)}{h^2} + O(h^2) \tag{14}$$

where h is the step size. Realistically, the wave functions should be defined from $\rho = [0, \infty)$, however, numerically we define a minimum value, $\rho_0 = 0$, and a maximum value, ρ_{max}, which will determine the step size for a given number of mesh points, N, as:

$$h = \frac{\rho_{max} - \rho_0}{N} \tag{15}$$

Using Equation 14, Equations 4 and 13 can be written as:

$$\left(\frac{2}{h^2} + V_i\right) u_i - \frac{1}{h^2} u_{i-1} - \frac{1}{h^2} u_{i+1} = \lambda u_i \tag{16}$$

where V_i is either ρ^2 for the non-interacting case, or $\omega_r^2 \rho^2 + 1/\rho$ for the interacting case. The above equation is an eigenvalue problem that can be written in matrix form as:

$$\begin{bmatrix} \frac{2}{h^2} + V_1 & -\frac{1}{h^2} & 0 \\ -\frac{1}{h^2} & \frac{2}{h^2} + V_2 & -\frac{1}{h^2} \\ 0 & -\frac{1}{h^2} & \frac{2}{h^2} + V_N \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_N \end{bmatrix} = \lambda \begin{bmatrix} u_0 \\ u_1 \\ u_N \end{bmatrix} \tag{17}$$

As an N dimensional matrix will have N eigenvalues and eigenvectors, the grid size necessarily determines the number of eigenvalues that will be produced. As we are only interested in the ground state and first two excited states, the minimum matrix size we can use is N = 3.

To begin the Jacobi algorithm we implement the vectors, v_i, and matrix, $\hat{a}$, using the Armadillo library [2]. The main premise is to diagonalize the matrix via repeated unitary transformations, given by $\hat{a}' = \hat{S}^T \hat{a} \hat{S}$, which take the largest non-diagonal matrix element to zero each iteration. This process continues until all off diagonal elements are less than the specified tolerance and thus are essentially zero. Once the diagonalization is complete, the eigenvalues are simply the values left on the diagonal.

For the eigenvectors we choose as a starting point unit vectors given by:

$$v_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad v_1 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad v_N = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{18}$$

Then for each iteration in the diagonalization scheme, the eigenvectors will undergo the same unitary transformation as the matrix, namely $v_i' = \hat{S} v_i$. As the transformation is unitary, the orthogonality of the eigenvectors will be preserved.

If the coordinates of the matrix element to be sent to zero are given by (k, l), the nonzero matrix elements of the rotation matrix, $\hat{S}$, are given by:

$$\begin{aligned} S_{(k,l)} &= -S_{(l,k)} = -sin(\theta) \\ S_{(k,k)} &= S_{(l,l)} = cos(\theta) \\ S_{(i,i)} &= 1 \quad i \neq k, i \neq l. \end{aligned} \tag{19}$$

After the transformation, the updated matrix elements of $\hat{a}'$ will be given by:

$$\begin{aligned} a'_{(k,l)} &= \left(a_{(k,k)} - a_{(l,l)}\right) cos(\theta) sin(\theta) + a_{(k,l)} \left(cos^2(\theta) - sin^2(\theta)\right) \\ a'_{(k,k)} &= a_{(k,k)} cos^2(\theta) - 2a_{(k,l)} cos(\theta) sin(\theta) + a_{(l,l)} sin^2(\theta) \\ a'_{(l,l)} &= a_{(l,l)} cos^2(\theta) + 2a_{(k,l)} cos(\theta) sin(\theta) + a_{(k,k)} sin^2(\theta) \\ a'_{(i,k)} &= a_{(i,k)} cos(\theta) - a_{(i,l)} sin(\theta) \quad i \neq k, l \\ a'_{(i,l)} &= a_{(i,l)} cos(\theta) + a_{(i,k)} sin(\theta) \quad i \neq k, l \end{aligned} \tag{20}$$

Since $a'_{(k,l)} \equiv 0$, $sin(\theta)$ and $cos(\theta)$ are determined via the expression above as:

$$cot(2\theta) \equiv \tau = \frac{a_{(l,l)} - a_{(k,k)}}{2a_{(k,l)}} \tag{21}$$

$$tan(\theta) = -\tau \pm \sqrt{1 + \tau^2} \tag{22}$$

$$cos(\theta) = \frac{1}{\sqrt{1 + tan^2(\theta)}} \tag{23}$$

$$sin(\theta) = tan(\theta) cos(\theta) \tag{24}$$

and the matrix elements are updated accordingly.

To determine the accuracy of our solutions, we define the average error as the average of the percentage differences of the first three energy eigenvalues calculated via the Jacobi algorithm, λ_n^j, as compared to their exact values, λ_n:

$$\epsilon_{avg} = \frac{1}{3} \left(\frac{|\lambda_0^j - \lambda_0|}{\lambda_0} + \frac{|\lambda_1^j - \lambda_1|}{\lambda_1} + \frac{|\lambda_2^j - \lambda_2|}{\lambda_2} \right) \tag{25}$$

III. RESULTS

IV. CONCLUSIONS

[1] M. Taut, Phys. Rev. A **48**, 3561 (1993).

[2] C. Sanderson and R. Curtin, *Armadillo: a template-based*

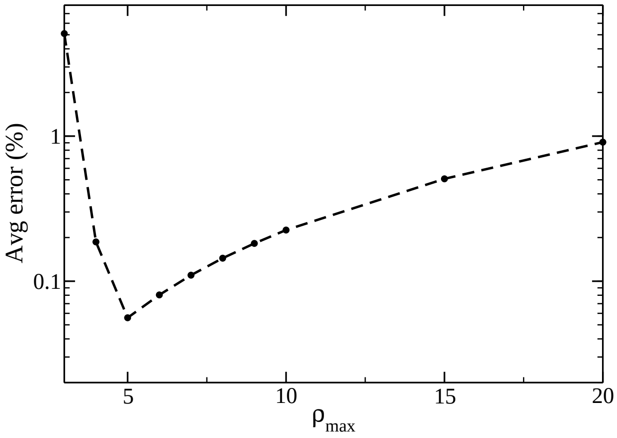

FIG. 1: error as a function of ρ_{max}

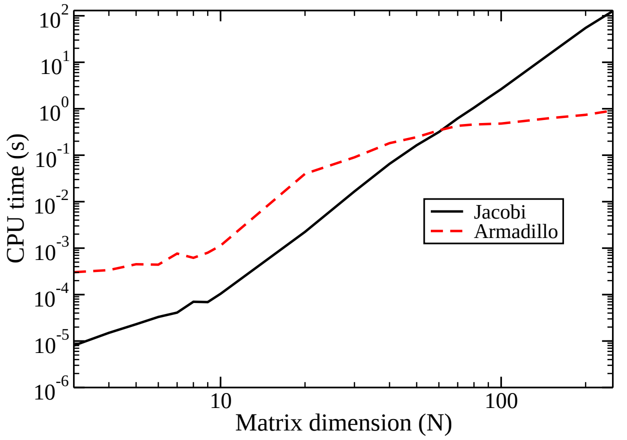

FIG. 2: time as a function of matrix dimension (N)

C++ library for linear algebra (????).

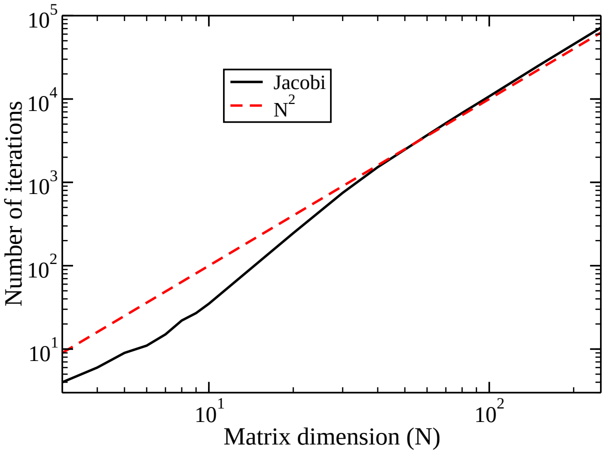

FIG. 3: number of rotations as a function of matrix dimension (N)

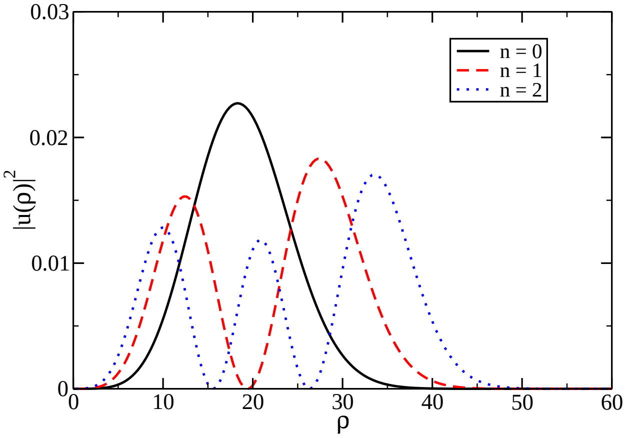

FIG. 4: $|u(\rho)|^2$ for $w_r = 0.01$

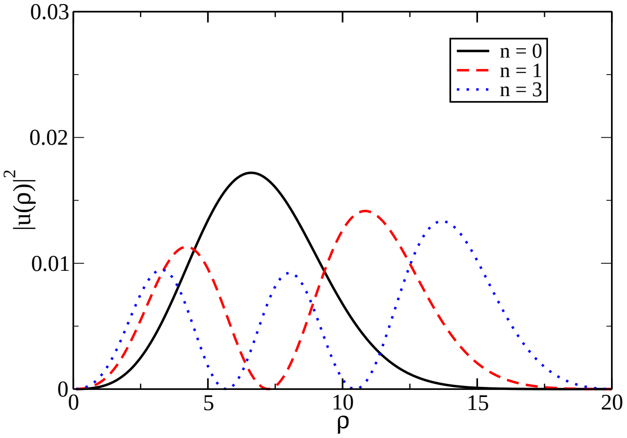

FIG. 5: $|u(\rho)|^2$ for $w_r = 0.05$

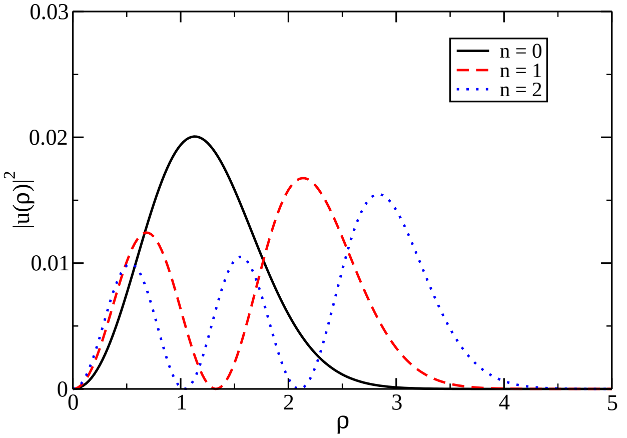

FIG. 6: $|u(\rho)|^2$ for $w_r = 1.0$

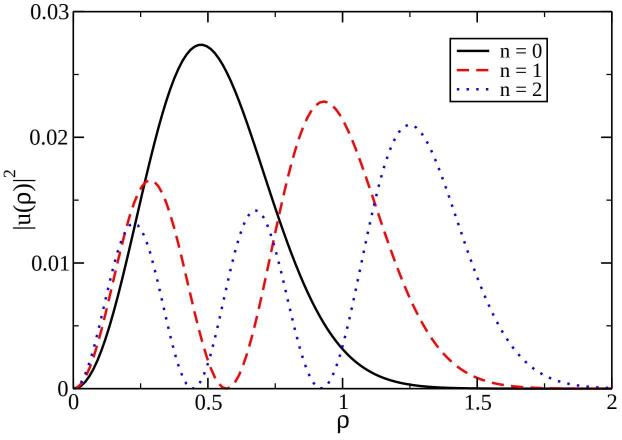

FIG. 7: $|u(\rho)|^2$ for $w_r = 5.0$