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:

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

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:

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

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:

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

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

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

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:

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

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:

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

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

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

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

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:

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

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

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

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

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:

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

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 $\lambda = m\alpha^2 E_r/\hbar^2$. Equation 12 then becomes:

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

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

III. RESULTS

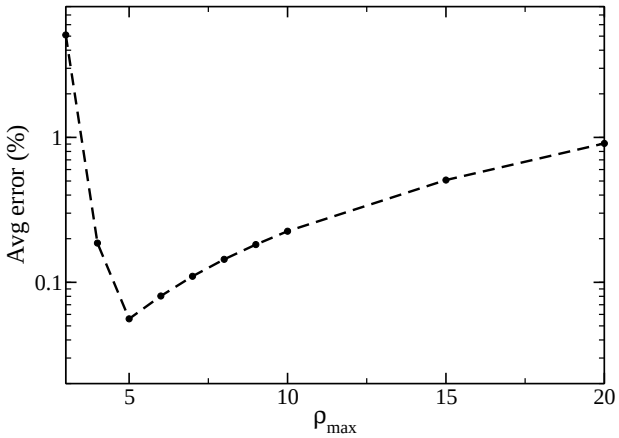

FIG. 1: error asa function of ρ_{max}

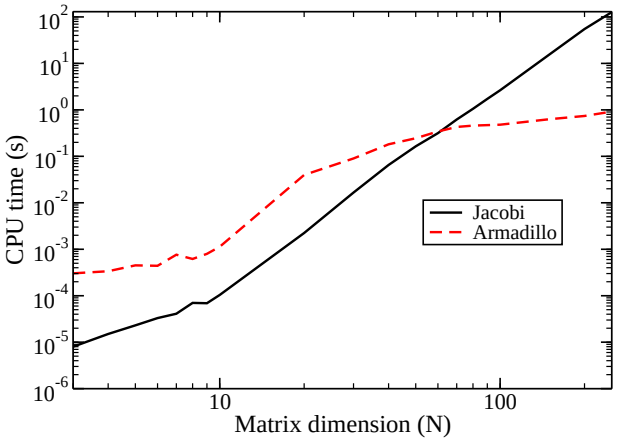

FIG. 2: time as a function of matrix dimension (N)

IV. CONCLUSIONS

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

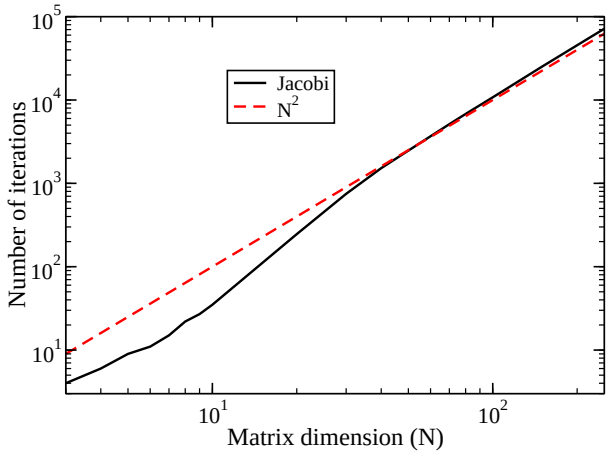

FIG. 3: number of rotations as a function of matrix dimension (N)

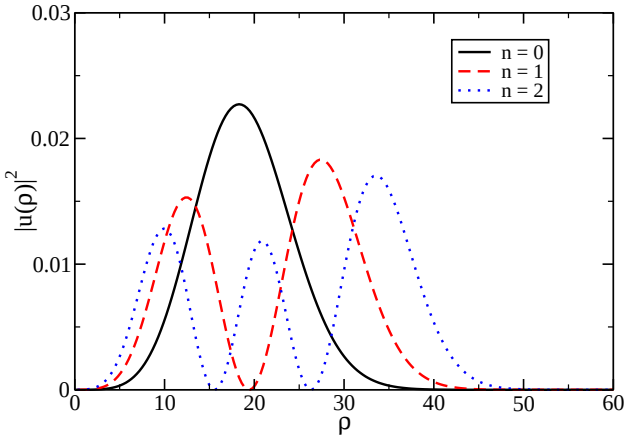

FIG. 4: $|u(\rho)|^2$ for $w_r = 0.01$

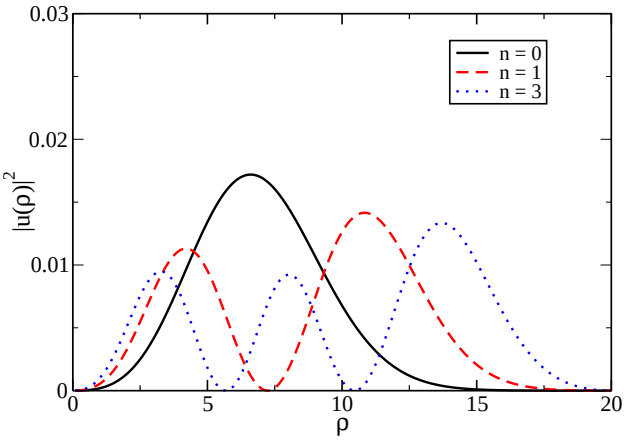

FIG. 5: $|u(\rho)|^2$ for $w_r = 0.05$

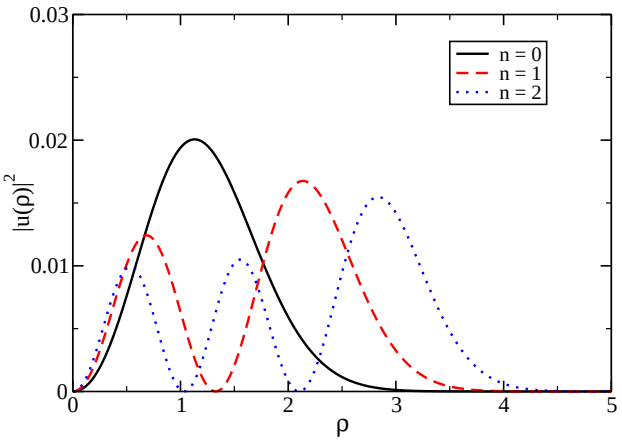

FIG. 6: $|u(\rho)|^2$ for $w_r = 1.0$

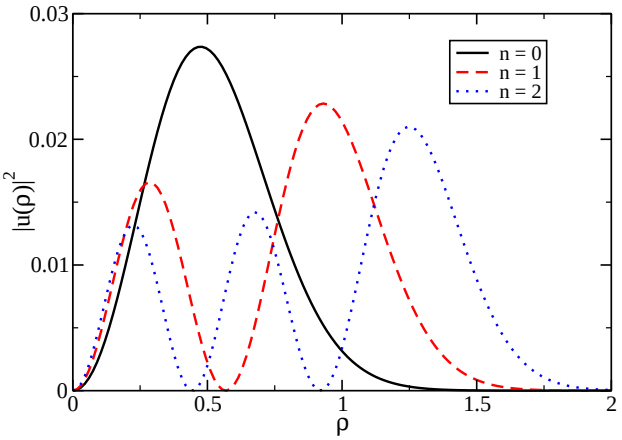

FIG. 7: $|u(\rho)|^2$ for $w_r = 5.0$