Project 1

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We present an algorithm that allows us to solve the Schrödinger equation for electron-electron interactions. Using Jacobi rotation methods, we are able to solve for the eigenvalues for a known potential equation. Using inherent eignenvalue solvers, we are able to verify the eigenvalues obtained through the Jacobi rotation methods. Comparisons between potential strengths provide insight on electron-electron interactions.

I. INTRODUCTION

One of the simplest cases of the Schrödinger equation comes from electron-electron interactions within a three-dimensional harmonic oscillator. To further simplify the problem, we can first solve for a case with no Coulomb interactions. Using multiple eigenvalue solvers (Jacobi rotations and built-in solvers) we are able to determine the eigenvalues resulting from a given Schrödinger equation. Analysis of the results provide insight on the effectiveness of the eigenvalue solvers.

II. THEORY, ALGORITHMS AND METHODS

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We begin our analysis by creating a simple test that allows us to verify the orthogonality preservation of the resulting eigenvalues.

III. ANALYSIS

A. Unit Tests

In order to verify the accuracy of the eigenvalue solvers, multiple tests were used. The first test that was used was an orthoganality preservation test. By taking two different eigenvectors of the diagonal matrix formed via the eigenvalue solvers, we would expect them to be orthogonal. Similarly, if we took identical eigenvectors we would expect a nonzero solution. These results are also portrayed by column vectors of a tri-diagonal matrix, including the one that was used to demonstrate the potential of the three-dimensional Schrödinger equation.

We set up a test that took two column vectors of the potential tridiagonal matrix and solved for the dot product. By calculating this, we verified that similar column vectors of the potential matrix produced a nonzero value (8.88 for a $N = 5$ matrix) and that non-similar column vectors produced zero.

We used this test after solving for the non-interacting case. We found that similar eigenvectors produced a nonzero value (8.62 for a $N = 5$ matrix) and non-similar eigenvectors produced zero.

We then used this test after solving for the interacting case. We found that non-similar eigenvectors produced zero while similar eigenvalues produced a non-zero solution (5.22 for a $N = 5$ matrix, while the potential matrix for this case yielded 3.03).

A second test was performed to check the accuracy of the Jacobi rotation eigenvalue solver. This test involved the use of small N matrices to compare to the c++ software package Armadillo [1].

B. Non-interacting Case

We began our analysis with a simple non-interacting form of the Schrödinger equation. By setting a simple potential, we are able to easily calculate and verify the eignevalues that are found via the Jacobi rotation method **??**. By setting a step length,

$$h = \frac{\rho_{max} - \rho_0}{N} \tag{1}$$

where ρ_{max} was set to 7.0, ρ_0 set to 0.0, and N the number of inputted mesh points, we should expect to find the same eignevalues for a given N.

Mesh Points (N)	Time$_{Jacobi}$ (sec)	Time$_{Armadillo}$ (sec)
2	0.00033	0.000044
5	0.00057	0.000087
8†	0.00107	0.000103
10	0.00136	0.000120
100	0.04778	0.001862

TABLE I: A time comparison between the Jacobi rotation and armadillo [1] eigenvalue solvers. The † represents the number of mesh points used to find the lowest three eigenvalues for the non-interacting case.

Using a N value of eight, we are able to find the first three lowest eigenvalues: 2.7405, 5.8654, and 9.6309. Using the Jacobi rotation method, we find that the matrix goes through N^2 similarity transformations to get a matrix with zero[1] non-diagonal matrix elements.

We were able to use Armadillo [1], to find the eigenvalues of the non-interacting case for the Schrödinger

[1] Zero to a certain approximation (i.e. 10^{-15} was set to zero).

equation to verify our results from the Jacobi rotation method. Both methods provided identical eigenvalues. Using both methods, we were able to calculate the amount of time required to carry out the calculations (Table III B).

C. Interacting Case

We then progressed to the Coulomb interaction case for the Schrödinger equation. We now find that we can solve for the same Schrödinger equation with a modified potential to account for the Coulomb interactions. The interaction potential was found to be directly proporational to a coefficienct, ω_r, that dictates strength of the oscillator potential. Using the found energy-eigenvalue relationship,

$$E = \frac{\hbar^2}{m\alpha^2}\lambda \tag{2}$$

where alpha is a fixed constant, we were able to determine the ground state energy for various ω_r (Table III C).

ω_r	$E^1_{GS}(J)$	$E^2_{GS}(J)$ [2]
0.01	0.11063	–
*0.05	0.12310	0.1750
*0.25	0.53431	0.6250
0.5	0.54408	–
1	0.96438	–
5	4.38549	–

TABLE II: Comparison between the ground state energy and ω_r. $E^1_{GS}(J)$ are ground state energies found in the present work and $E^2_{GS}(J)$ are accepted values found in Ref. [2]. The * indicates ω_r values that overlap with the accepted values in Ref. [2]. In order to get a good approximation to the accepted value, the ground state energy for $\omega_r = 0.25$ was found using the second lowest eigenvalue.

[1] C. Sanderson and R. Curtin, Journal of Open Source Software **1**, 26 (2016).

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