MTH 480 Project 2

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1 Abstract

2 Introduction

Last time we took the Schrödinger equation and transformed it to the radial equation in center of mass frame.

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

we are only interested in the

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

we can make the equation dimensionless which gives

$$\left(-\partial_\rho^2 + \rho^2 + \frac{\beta}{\rho}\right)u(\rho) = \lambda u(\rho) \left(-\partial_\rho^2 + V(\rho)\right)u(\rho) = \lambda u(\rho) \tag{3}$$

Discretize

$$\begin{aligned} u(\rho) &\to u(\rho_i) = u_i \\ \rho &\to \rho_i = \rho_0 + ih \\ h &= \frac{b-a}{n+1} \\ a &= 0 \end{aligned} \tag{4}$$

the linear algebra equation is

$$\hat{A} = \begin{pmatrix} \frac{2}{h^2} + V_1 & -\frac{1}{h^2} & & & \\ -\frac{1}{h^2} & \frac{2}{h^2} + V_2 & -\frac{1}{h^2} & & \\ & & \ddots & & \\ & & & & -\frac{1}{h^2} \\ & & & -\frac{1}{h^2} & \frac{2}{h^2} + V_{N-1} \end{pmatrix} \tag{5}$$

$$\hat{A}x = \lambda x \tag{6}$$

$$S^T A x = \lambda S^T x \tag{7}$$

$$S^T A S (S^T x) = \lambda (S^T x) \tag{8}$$

Eigenvalues unchanged under orthogonal transforms
Eigenvectors change, but the length is preserved
Dot product between vectors is conserved

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 1: rhoMax = 5.0

3 Methods

We performed a Jacobian eigenvalue algorithm to

4 Analysis

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

4.1 Part B

5 Conclusions

6 Works Cited