Project 2 - working title

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I. INTRODUCTION

Differential equations (DEs) show up in all branches of physics, and many of them can be recast into a eigenvalue problem.

II. METHOD

A. A Buckling Beam problem

We'll first study the differential equation of the form

$$\gamma \frac{\mathrm{d}^2 u(x)}{\mathrm{d}x^2} = -Fu(x), \tag{1}$$

which essentially is a 1-dimensional wave equation. Assume here that $x \in [0, L]$ for some known length L and suppose we know the exact value of F. Defining a new variable $\rho \equiv x/L$,, we can recast the DE as

$$\frac{\mathrm{d}^2 u(\rho)}{\mathrm{d}\rho^2} = -\frac{FL^2}{\gamma} u(\rho) \equiv -\lambda u(\rho), \tag{2}$$

where $\rho \in [\rho_0, \rho_N] = [0, 1]$. We can discretize the second derivative here as

$$\frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}, \tag{3}$$

where $u_i \equiv u(\rho_i)$, $\rho_i \equiv \rho_0 + ih$ for $i = 1, 2, .., N$ for N grid points and some step size h. Then equation (2) can be written as

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = -\lambda u_i \tag{4}$$

Eq. (4) can easily be recast into the following matrix equation.

$$\frac{1}{h^2}\begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{bmatrix} \tag{5}$$

Quantum dots in 3D - one electron

Here we'll study Schrödinger's equation for one electron. The radial equation of any spherically symmetric potential $V(r)$ can be written as

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 u(r)}{\mathrm{d}r^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right] u(r) = Eu(r), \tag{6}$$

where the radial function $R(r)$ is related to the eq. (6) by the definition $u(r) \equiv rR(r)$. In this article we'll restrict ourselves to the case $\ell = 0$, that is, the electron has no angular momentum. To recast this equation into a simpler form, we'll define $\rho \equiv r/\alpha$ where α is some parameter with units length. Then eq. (6) can be rewritten as

$$-\frac{\mathrm{d}^2 u(\rho)}{\mathrm{d}\rho^2} + \rho^2 u(\rho) = \lambda u(\rho), \tag{7}$$

as derived in the appendix (MAKE THIS DERIVATION LATER). Here $\alpha \equiv (\hbar^2/mk)^{1/4}$ and $\lambda \equiv (2m\alpha^2/\hbar^2)E$. The boundary conditions here are $u(0) = 0$ and $u(\infty) = 0$, which follows from the requirement that the resulting radial function must obey $\int r^2|R(r)|dr < \infty$ such that $R(r) \in L^2(0, \infty)$ and is thus normalizable. Discretization of eq. (7) in the same manner as done with the buckling beam equation, we obtain

$$\frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} + \rho_i^2 u_i = \lambda u_i, \tag{8}$$

which we can easily recast into a matrix equation as follows.

$$\frac{1}{h^2}\begin{bmatrix} U_1 & -1 & 0 & \cdots & 0 \\ -1 & U_2 & -1 & \cdots & 0 \\ 0 & -1 & U_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -1 & U_{n-1} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_{n-1} \end{bmatrix}, \tag{9}$$

where we define $U_i \equiv 2 + \rho_i^2 h^2$.

Quantum dots in 3D - two electrons

B. Algorithm

C. Important mathematical properties

1. *Unitary transformations conserve orthonormality*

Suppose A is a symmetric matrix and S is a unitary matrix, such that $S^\dagger S = SS^\dagger = 1$. Suppose further that $\{\boldsymbol{v}_i\}$ are a orthonormal set of eigenvectors of A. It then follows that

$$\begin{aligned} \langle S\boldsymbol{v}_i, S\boldsymbol{v}_j\rangle &= (S\boldsymbol{v}_i)^\dagger (S\boldsymbol{v}_j) = \boldsymbol{v}_i^T(S^\dagger S)\boldsymbol{v}_j \\ &= \langle \boldsymbol{v}_i, \boldsymbol{v}_j\rangle = \delta_{ij}, \end{aligned} \tag{10}$$

where δ_{ij} is the Kronecker delta.

2. Similar matrices share eigenvalue spectrum

Suppose B is similar to A, that is $B = S^T AS$ for a real unitary matrix S. We prove here that B has the same eigenvalues as A. Let $\boldsymbol{v}_i$ have the corresponding eigenvalue λ_i, then

$$B(S^T \boldsymbol{v}_i) = S^T A\boldsymbol{v}_i = \lambda_i (S^T \boldsymbol{v}_i), \tag{11}$$

which proves that B has eigenvalues λ_i with corresponding eigenvectors $S^T \boldsymbol{v}_i$.

3. The eigenvectors a similar matrix is orthogonal

Suppose $B = S^T AS$ and A is symmetric, then

$$B^T = \left(S^T AS\right)^T = S^T A^T (S^T)^T = S^T AS = B, \tag{12}$$

By the spectral theorem for symmetric matrices, it then follows that the eigenvectors of B are orthogonal as long as they span different eigenspaces.

III. RESULTS

IV. DISCUSSION

V. CONCLUSION