

# 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 an eigenvalue problem.

## II. METHOD

### A. A Buckling Beam problem

We'll first study the differential equation of the form

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

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

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

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

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

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

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

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

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

### 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

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

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  $\alpha$  is some parameter with units length. Then eq. (6) can be rewritten as

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

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

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

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

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

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  $\{\mathbf{v}_i\}$  are an orthonormal set of eigenvectors of  $A$ . It then follows that

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

where  $\delta_{ij}$  is the Kronecker delta.

2. *Similar matrices share eigenvalue spectrum*

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

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

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

3. *The eigenvectors a similar matrix is orthogonal*

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

$$B^T = (S^T A S)^T = S^T A^T (S^T)^T = S^T A S = B, \quad (12)$$

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