Project 1

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I. PART I

A.

Here, we are trying to solve for the solutions to Schrodinger's eigenvalue equation:

$$\hat{H}_0\phi_n = \epsilon_n\phi_n$$

By discretizing ϕ_n, each ϕ_n becomes a finite dimensional vector and we can write $\hat{H}$ explicitly as a matrix. That matrix satisfies

$$\sum_j \langle i| \hat{H}_0 |j\rangle \vec{\phi}_{n,j} = \epsilon_n\vec{\phi}_n$$

wheree $\langle i| \hat{H}_0 |j\rangle$ is the matrix element $[H_0]_{ij}$. It was shown the Schrodingers wave equation could be expressed in discrete form, as

$$-t(\phi_{n,i+1} + \phi_{n,i-1}) + (2t + V_i)\phi_{n,i} = \epsilon_n\phi_{n,i}$$

which gives us a relationship between $\phi_{n,i}$ and the neighboring elements $\phi_{n,i-1}$ and $\phi_{n,i+1}$. The eigenvalues equation can then be written as a matrix multiplication

$$\hat{H}_0\phi_n = \begin{pmatrix} 2t+V_1 & -t & 0 & \dots \\ -t & 2t+V_2 & -t & \dots \\ 0 & -t & 2t+V_3 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \phi_{n,1} \\ \phi_{n,2} \\ \phi_{n,3} \\ \vdots \end{pmatrix} \quad (1)$$

The full matrix $\hat{H}_0$ is shown in Figure 1a.

B.

From (1) we can see that the diagonal elements represent the discretized potential V_n (plus a constant $2t$ where $t = \frac{\hbar^2}{2ma^2}$). The off-diagonal elements are just constants with dimension of energy over length squared. The matrix of normalized eigenvectors of $\hat{H}_0$ are shown in Figure 1b.

C.

To show that the eigenvectors form an orthonormal set, We can define a matrix T such that each column of T is one eigenvector $\vec{\phi}_n$ of $\hat{H}_0$. If the eigenvectors are indeed orthonormal, then

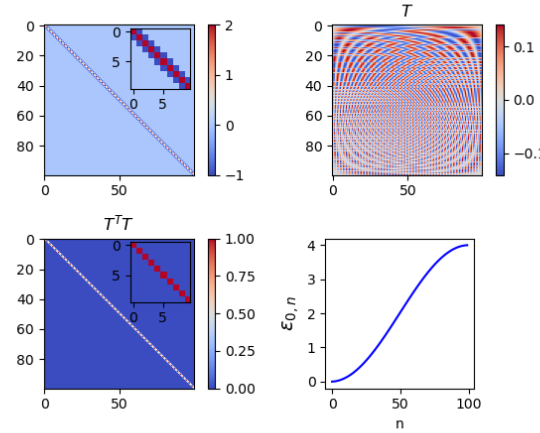

FIG. 1. The Hamiltonian matrix for $t = 1$

$$T^T T = I$$

This product is shown in Figure 1c, and we can see that the eigenvectors are orthonormal.

D.

The eigenvalues ϵ_n are shown in Figure 1d in ascending order, indexed by n.

E.

The probability distributions $|\langle n|\phi\rangle|^2$ for eigenvectors $n = 0, 10, 50$ are shown in the position represention in Figure 2.

F.

The standard quantum mechanics problem this corresponds to is the free particle in zero potential:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$$

$$\frac{\partial^2\psi}{\partial x^2} = -k^2\psi$$

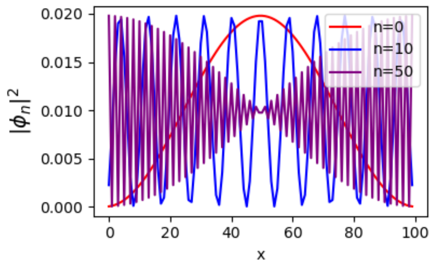

FIG. 2.

for $k = \frac{\sqrt{2mE}}{\hbar}$. So clearly the energy eigenvalues are $E_k = \hbar k^2/2m$. Notice that k is a continuous parameter and therefore there is a continuum of solutions to the eigenvalue equation. The general solution to the above equation is

$$\psi(x) = Ae^{ikx}$$

We would expect that the energy eigenvalues in Figure 1d would vary quadratically in n; however, the curve has a more sigmoidal shape. Around $n = 50$, we can see that the eigenvalues are increasing more linearly because those solutions are actually superpositions of harmonics (See Figure 2, $n = 50$ in purple).

II.

To understand why, notice that another perfectly valid solution of Schrodinger's equation is

$$\begin{aligned}\psi(x) &= Ae^{ikx} + Be^{ik'x} \\ &= e^{i(k+k')x/2}\left(Ae^{i(k-k')x/2)} + Be^{-i(k-k')x/2}\right)\end{aligned}$$

which is a wave with frequency $k - k'$ modulated by the average frequency $(k + k')/2$. Furthermore, eigenvalue curve plateaus as $n \to 100$ because we have chosen a finite sampling frequency a, and higher energy solutions cannot be resolved.

III.

The unitary operator that transforms $\hat{H}_0$ into the $|n\rangle$ basis to the $|\phi_n\rangle$ basis is simply

$$U_0 = T^{-1}$$

which we can use to represent our Hamiltonian in the energy basis (we are just diagonalizing the Hamiltonian)

$$\hat{H} = U_0 H_0 U_0^{-1}$$

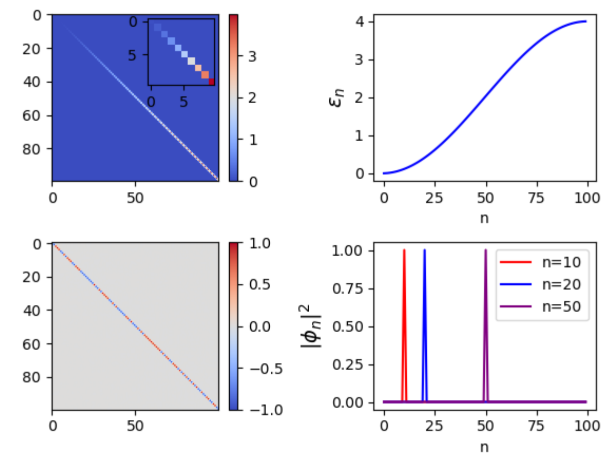

FIG. 3.

$\hat{H}$ is shown in Figure 3a, and is diagonal. Of course, this means that the matrix of eigenvectors T is also now a diagonal matrix. The values along the diagonal are ± 1 since the vectors were already shown to be orthonormal and U_0 was a unitary matrix and therefore preserves orthonormality. The values along the diagonal are ± 1 because there is a phase. Example probability mass functions $|\phi_n|^2$ are shown in Figure 3d, and are delta functions $\delta(n - n')$, since we have transformed to the energy basis.