Project 1

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I. PROJECT 1

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

$$T^T T = I$$

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

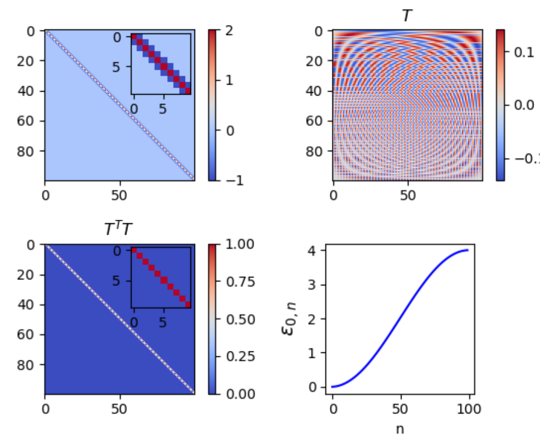

FIG. 1. The Hamiltonian matrix for $t = 1$

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:

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

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

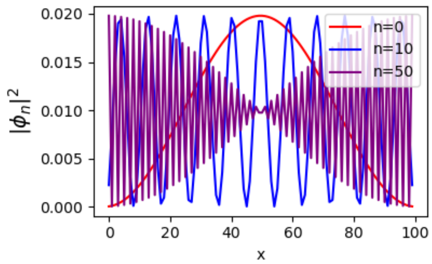

FIG. 2.

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).

G.

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.

H.

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)

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

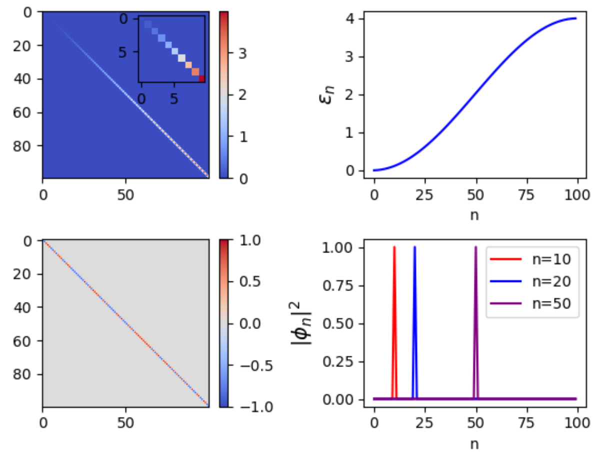

FIG. 3.

$\hat{H}$ 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.

I.

$\hat{H}$ differs from $\hat{H}_0$ from zero to the 29th element and the 69th element to the 100th element along the diagonal. This is because we have set $V = V_L$ for $0 \leq x \leq 29a$ and $V = V_R$ for $69a \leq x \leq 100$. The matrix $\hat{H}$ is shown in Figure 1a, its sorted eigenvectors are shown in Figure 4b, and their corresponding eigenvalues, sorted in ascending order, are shown in Figure 4d.

For $n = 0$ a particle is most likely to be in the region where $V = 0$, which makes sense because this is the ground state. As we increase the energy for $n = 24, 25, 34$, we see that the particle is no longer bound to the potential well ($E > V_L$), but it doesn't have enough energy to be found from $69a \leq x \leq 100$ where $V = V_R$ (($E < V_R$). So we see decaying exponenitals there. Furthermore, for $n = 38, 40, 54, 55$ we see sinusoidal solutions in both regions $0 \leq x \leq 29a$ and $69a \leq x \leq 100$. Clearly the energy is then high enough for the particle to be found there ($E > V_R$).

There are kinks in the energy eigenvalue plot because neighboring eigenvectors have more similar energy eigenvalues than before. Presumably this is because the asymmetric shape of the promotes a more discontinuous eigenvalue spectrum.

The eigenvalue plot for $U_0 H U_0^{-1}$ is the same as for H, as they should be. Just because we have changed our

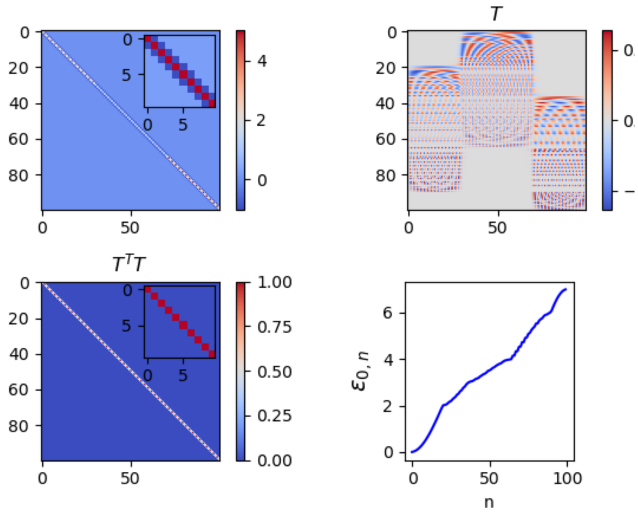

FIG. 4.

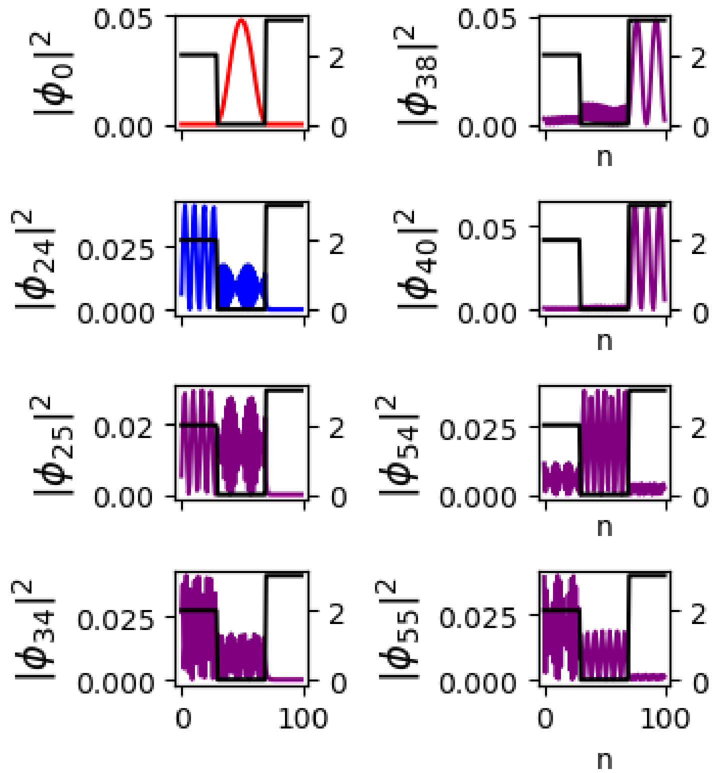

FIG. 5. Eigenvectors of the Hamiltonain

representation doesn't change anything physical about the system.

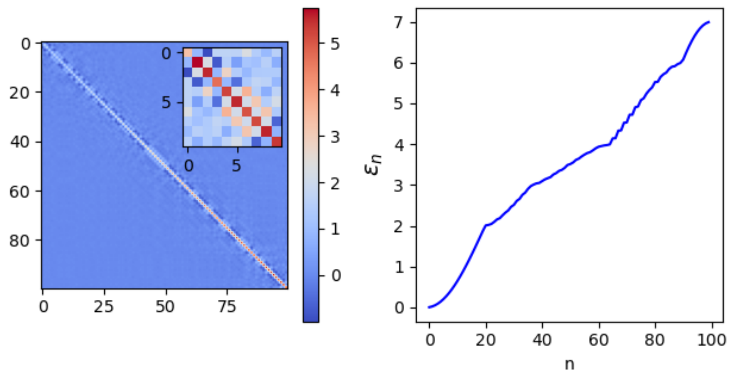

FIG. 6. Unitary transformation of H using U_0

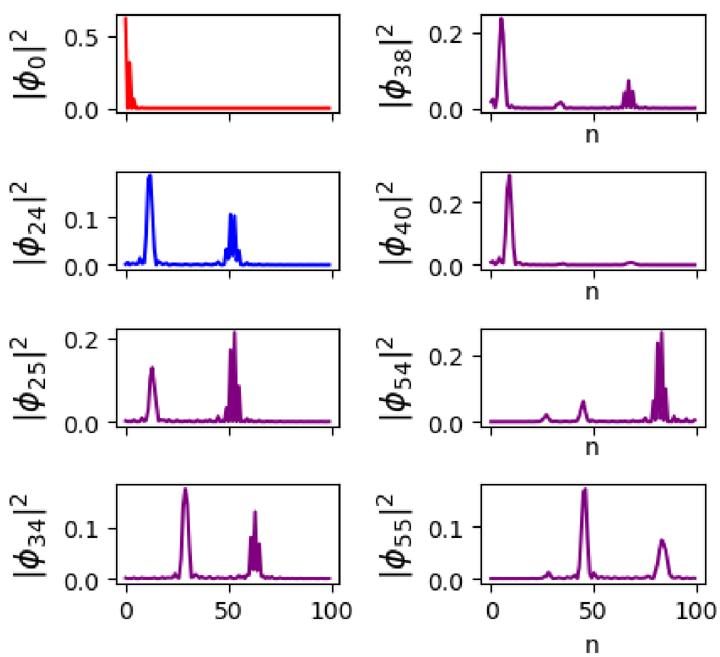

FIG. 7. Eigenvectors of H in H_0 eigenvector basis