Project 1

Quantum Mechanics
October 30, 2022 C Seitz

Part 1

A

We were given the Hamiltonian:

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

which gives us a relationship between $\phi_{n,i}$ and the neighboring elements $\phi_{n,i-1}$ and $\phi_{n,i+1}$. The explicit matrix form is

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

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

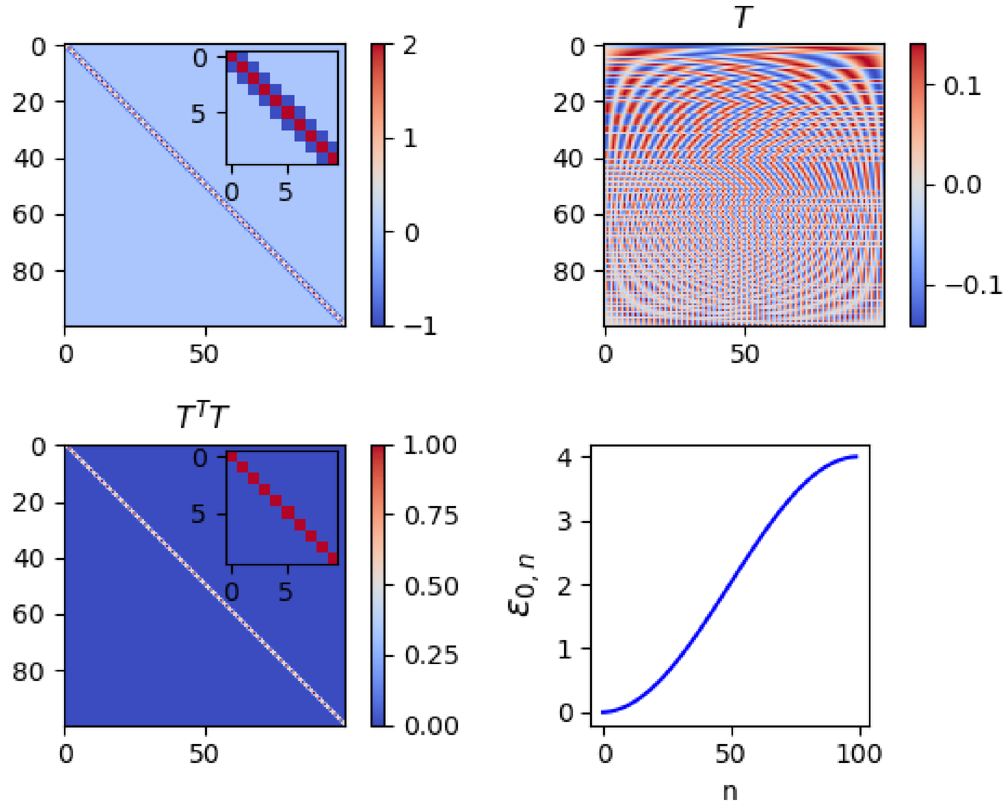

Figure 1: The Hamiltonian matrix for $t = 1$

$$T^T T = I$$

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

D

The sorted eigenvalues are shown in Figure 1d.

E

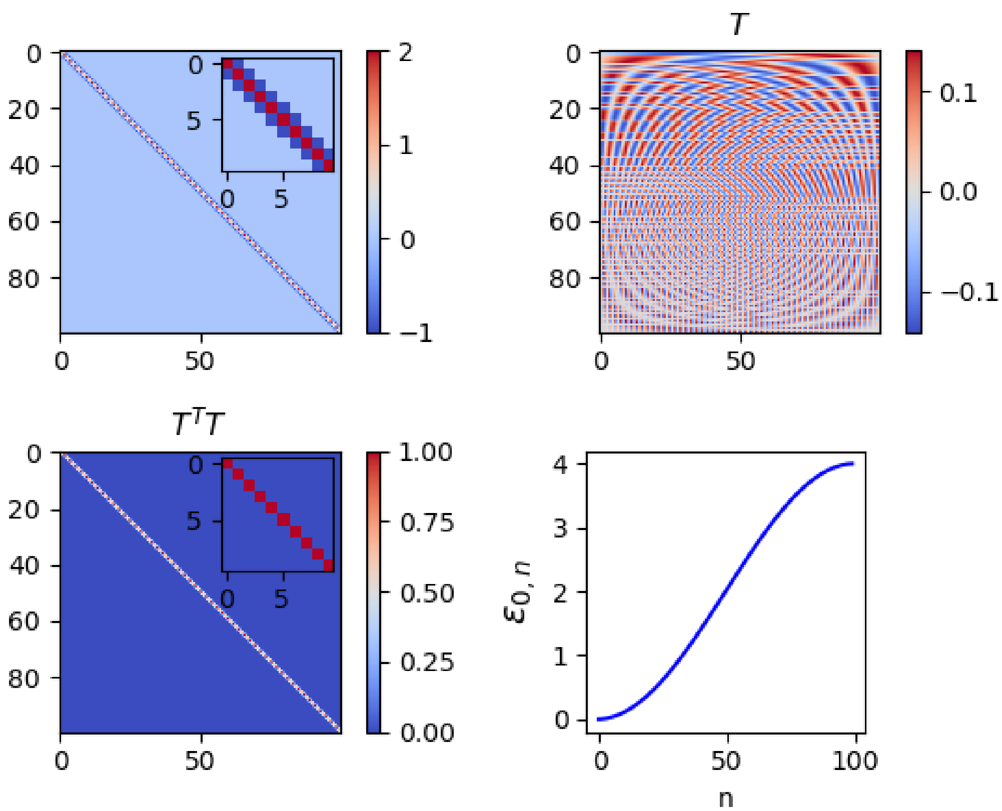

Figure 2: The Hamiltonian matrix for $t = 1$