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

$$T^T T = I$$

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

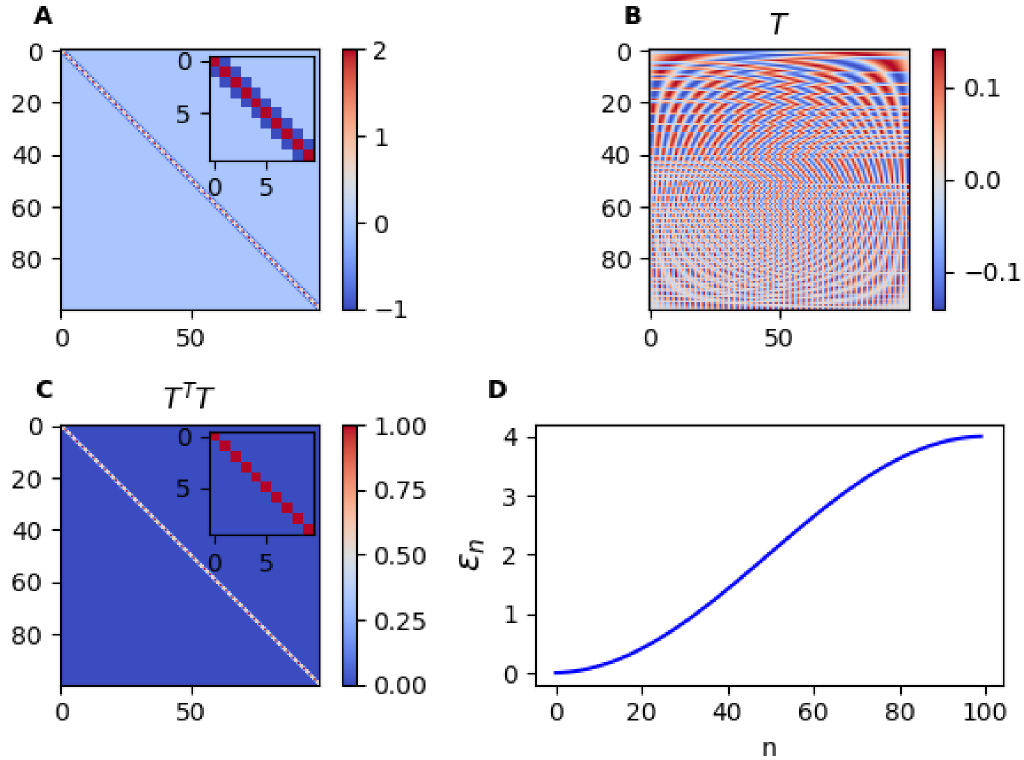

Figure 1: (A) The Hamiltonian H_0 (B) Eigenvectors as columns of a matrix (sorted by ascending eigenvalue) (C) Eigenvalue spectrum sorted in ascending order

(D) The sorted eigenvalues are shown in Figure 1d.

(E) Three example probability distributions are shown in Figure 2

(F) The standard quantum mechanics problem this corresponds to is the free particle.

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

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

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

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

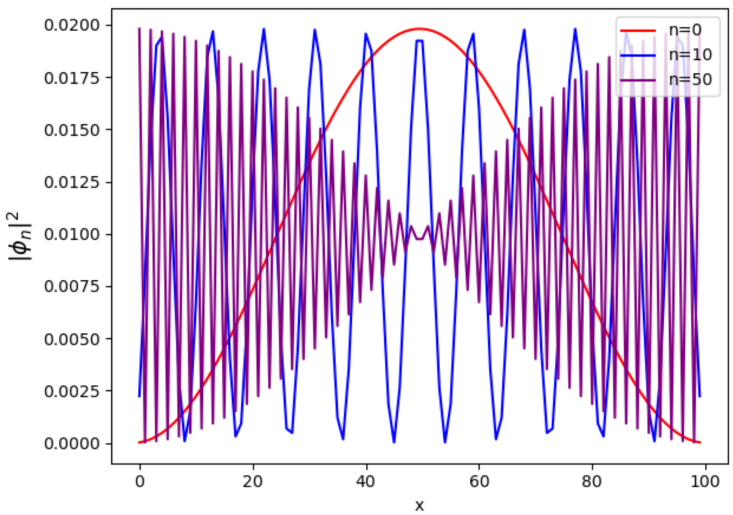

Figure 2: Energy eigenkets in the position representation for $n = 0, 10, 50$

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 there are beats (for example see $n = 50$), 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)

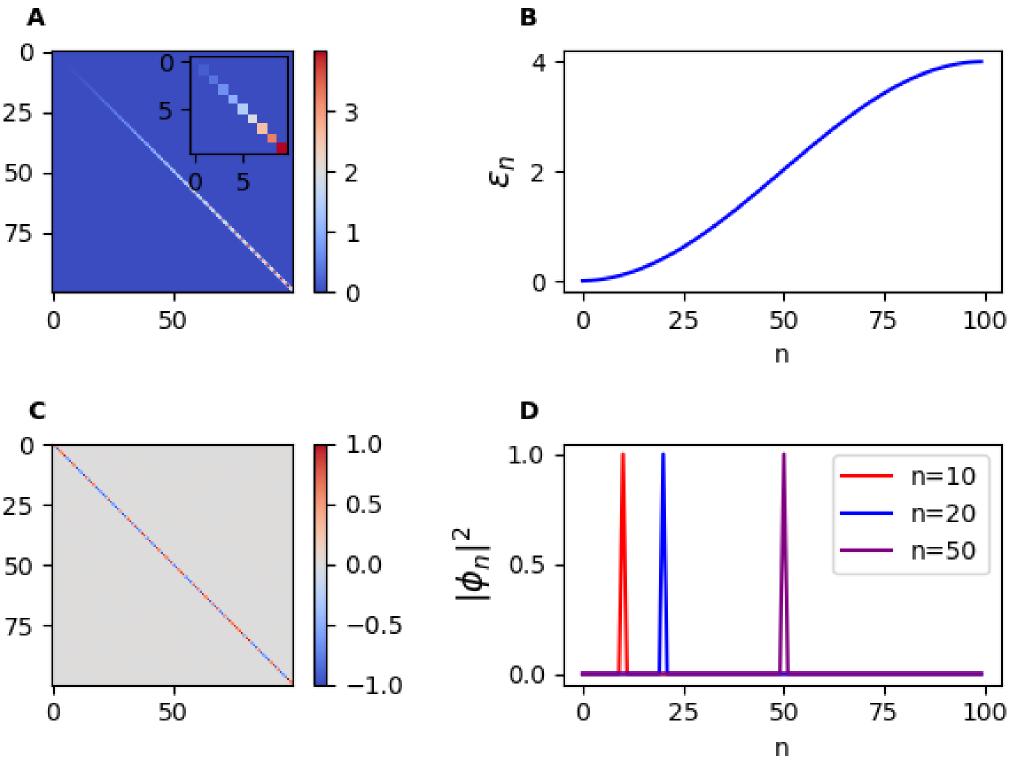

Figure 3: (A) The Hamiltonian H_0 after unitary transformation with U_0 (B) Eigenvalue spectrum sorted in ascending order (C) Eigenvectors as columns of a matrix (sorted by ascending eigenvalue) (D) Probability densities for a few eigenvectors in the energy basis

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

$\hat{H}$ is shown in Figure 3a, and is diagonal.

(I) The values along the diagonal of $\hat{H}$ are the energy eigenvalues

(J) The energy eigenvalues are shown in Figure 3b

(K) The energy eigenvalues are the same as they were before the change of basis. All we have done is changed our representation, so they should be.

(L) Three representative probability distributions are shown in Figure 3d. These are delta functions because we have changed to the energy basis.

Part 2

(M) The Hamiltonian matrix is shown in Figure 4a.

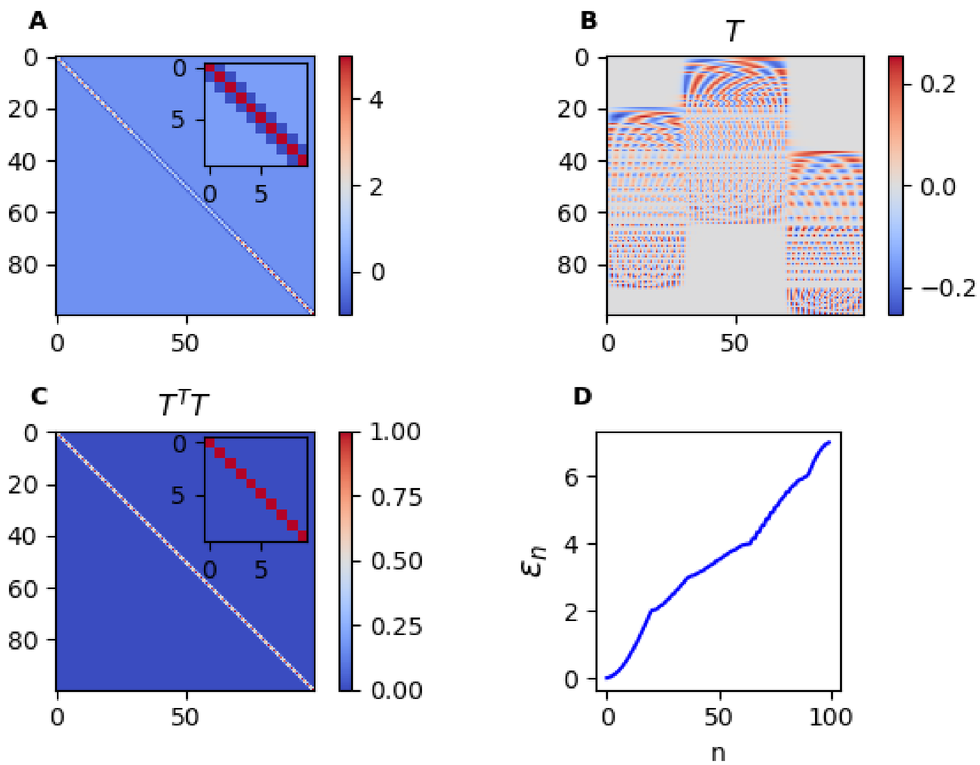

Figure 4: (A) The Hamiltonain H (B) Eigenvalue spectrum sorted in ascending order (C) Eigenvectors as columns of a matrix (sorted by ascending eigenvalue)

(N) $\hat{H}$ 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.

(O) The energy eigenvalues for this Hamiltonian are shown in Figure 4d.

(P) Probability distributions for $n = 1, 25, 26, 35, 39, 41, 55$ are shown in Figure 5.

(Q) 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

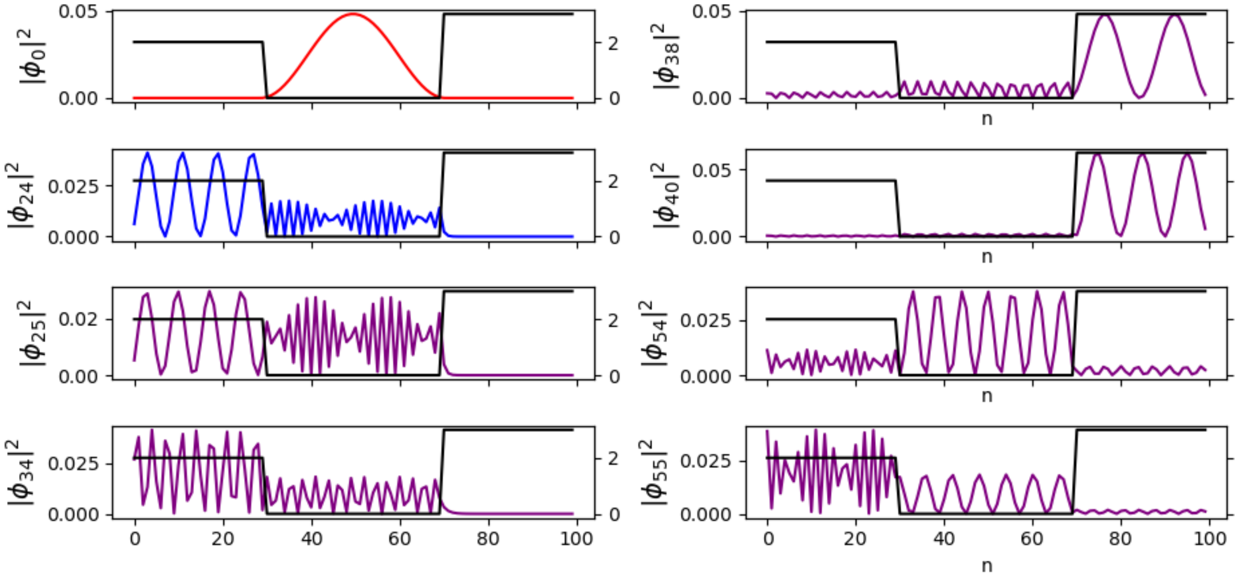

Figure 5: Probability densities for a few eigenkets of H

enough for the particle to be found there ($E > V_R$).

(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.

(S) The matrix after unitary transformation is shown in Figure 6a.

(T)

(U) The eigenvalue plot for $U_0 H U_0^{-1}$ is the same as for H, as they should be. Again, we have changed our representation but nothing physical has changed.

(V) The probability distributions $|\langle\phi_{0,m}|\phi_n\rangle|^2$ for $n = 1, 25, 26, 35, 39, 41, 55$ are shown in Figure 7.

(W) Let $|\phi_n\rangle$ be an orthonormal set of energy eigenkets of $\hat{H}$ and $|\phi_m\rangle$ be an orthonormal set of eigenkets of $\hat{H}_0$. Then $\sum_m |\phi_m\rangle\langle\phi_m|\phi_n\rangle$ is the representation of $|\phi_n\rangle$ in the $|\phi_m\rangle$ basis. It follows that $|\langle\phi_m|\phi_n\rangle|^2$ is the norm squared of that representation. Ultimately, we see spikes because for certain m, because $\langle\phi_n|\phi_n\rangle$ has greater magnitude.

(X) The matrix of values $\langle\phi_m|\phi_n\rangle$ is shown in Figure 6c. Each column of this matrix is an eigenvector $|\phi_n\rangle$ in the $|\phi_m\rangle$ basis. We can see that the kets $|\phi_n\rangle$ are superpositions of the plane wave solutions to the free particle

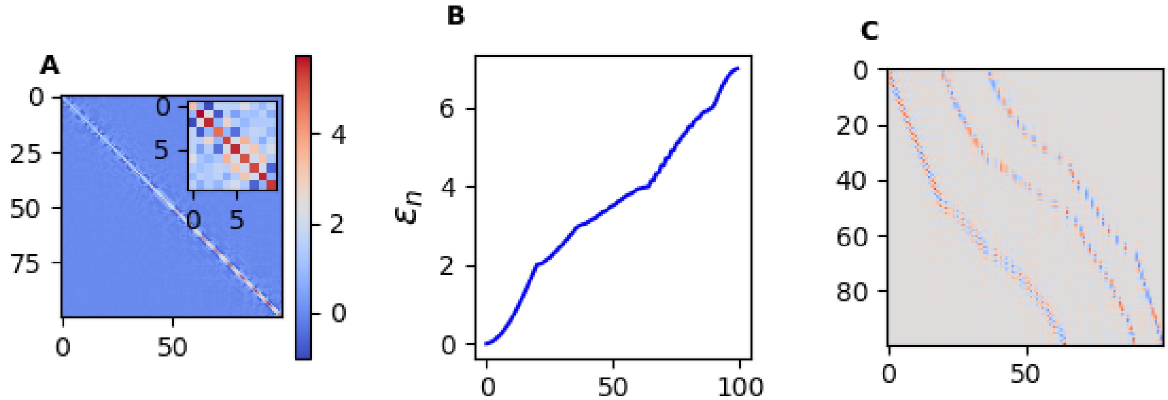

Figure 6: (A) The Hamiltonain after unitary transformation with U_0 (B) Eigenvalue spectrum sorted in ascending order (C) Eigenvectors as columns of a matrix (sorted by ascending eigenvalue)

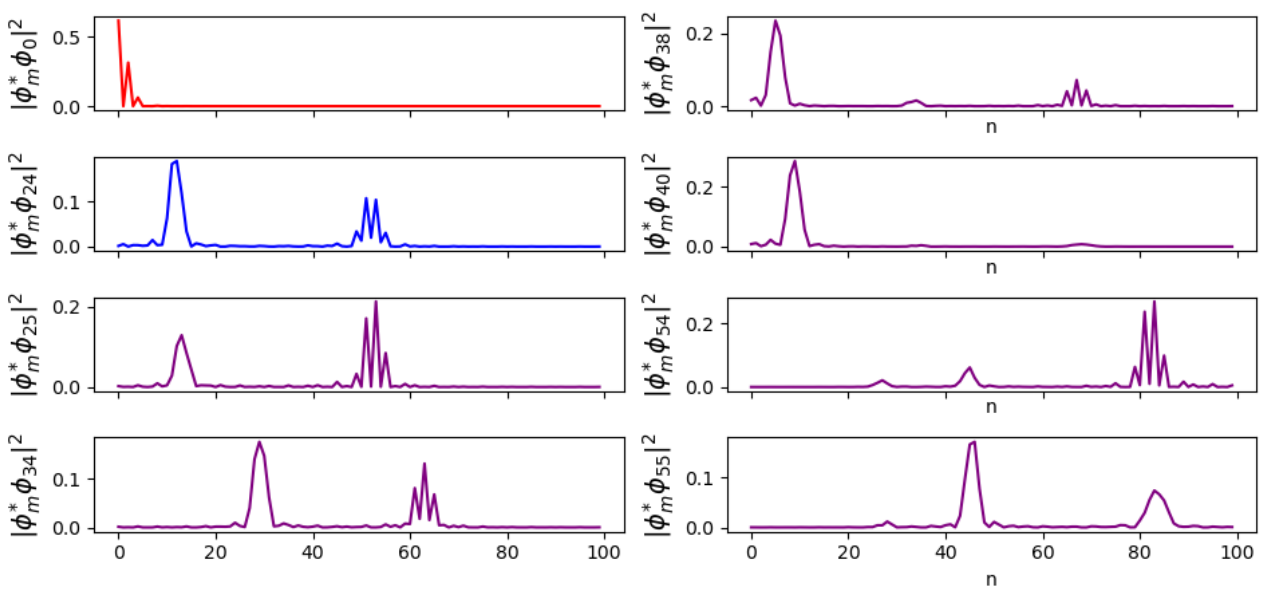

Figure 7: Representative probability distributions for eigenvectors of H in H_0 eigenbasis

problem. This makes sense, because using Fourier analysis, we should be able to construct arbitrary wavefunctions using a basis consisting of fundamental harmonics.