Homework 6 Write-Up

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1. EXERCISE 6.9 ASYMMETRIC QUANTUM WELL

For this exercise, we were asked to calculate the eigenvalues (E), eigenvectors (ψ), and the probability density for an asymmetric quantum well. First, we were asked to prove an equation from the given Equation 1 and Equation 1 and my calculations can be seen in Figure 1. Then we were asked to show that Schrodinger's equation can be written in matrix form (as seen in Figure 2). This shows that the eigenvalues of the matrix H are actually the allowed energies of the partibles in the well.

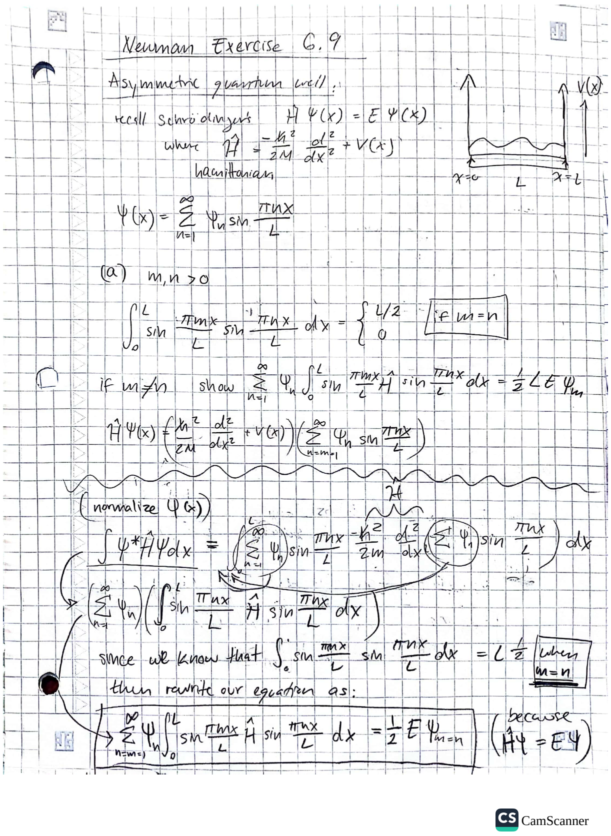

FIG. 1: Calculations for 6.9 Newman (A) Part 1.

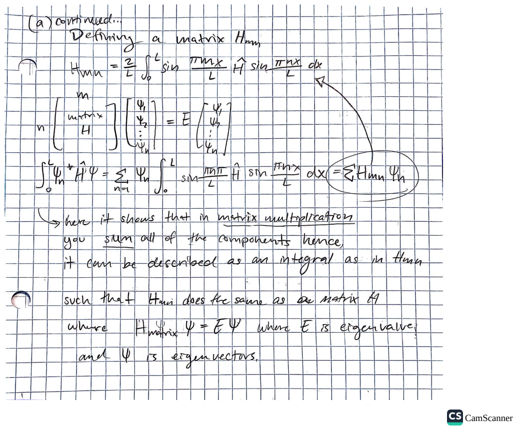

FIG. 2: Calculations for 6.9 Newman (A) Part 2.

$$\hat{H} = \frac{\hbar^2}{2M}\frac{d^2}{dx^2} + V(x) \tag{1}$$

$$\psi(x) = \sum_{n=1}^{\infty} \psi_n sin\frac{\pi n x}{L} \tag{2}$$

In Part (B) of this exercise, we used Equations 1,1, 1 to solve for the general solutions for matrix elements $H_m n$ which resulted in the solutions in Equation 1 and calculations can be seen in Figure 3. The rest of the exercise in outlined in Figure 4.

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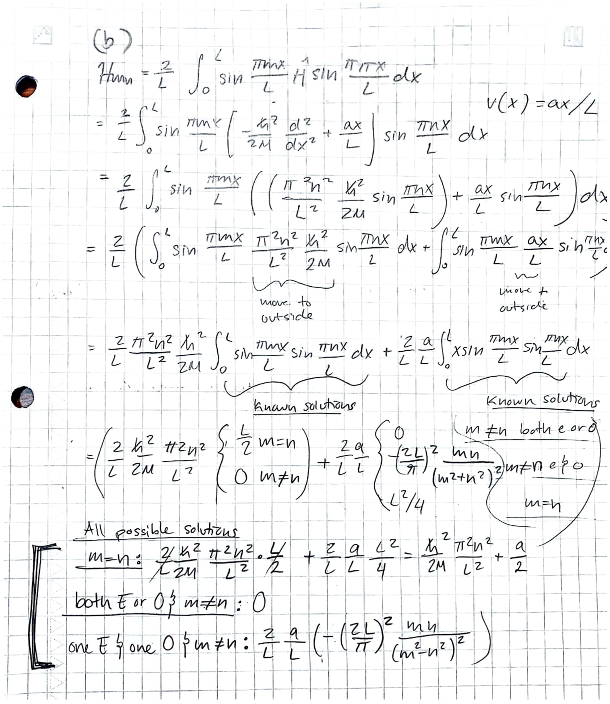


FIG. 3: Finding general expression for matrix element H_{mn} Part (B).

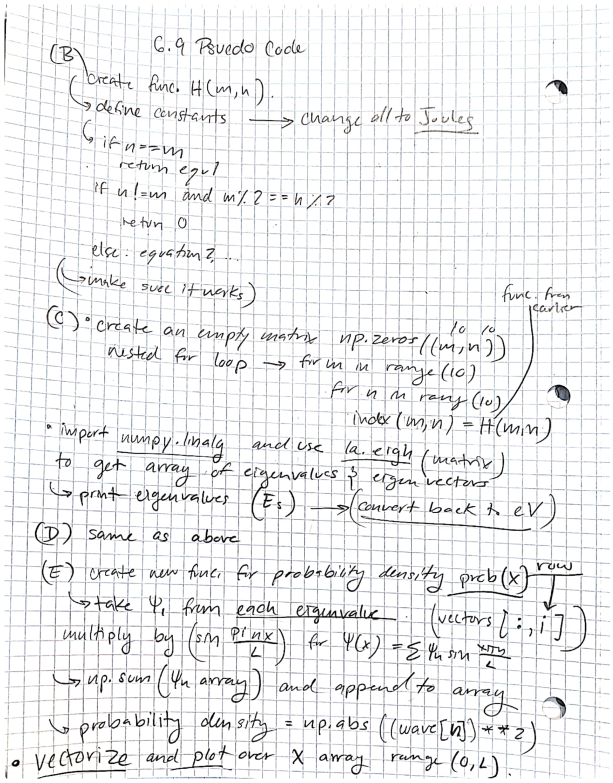


FIG. 4: Pseudo code for Exercise 6.9 Newman.

$$H_mn = \frac{2}{L}\int_0^L sin\frac{\pi m x}{L}\hat{H}sin\frac{\pi n x}{L}dx \tag{3}$$

$$\int_0^L sin\frac{\pi m x}{L}sin\frac{\pi n x}{L}dx = \begin{cases}\frac{L}{2} & \text{if } m = n\\ 0 & \text{otherwise}\end{cases} \tag{4}$$

$$\int_0^L xsin\frac{\pi m x}{L}sin\frac{\pi n x}{L}dx = \begin{cases}\frac{L^2}{4}\\ -(\frac{2L}{\pi})^2\frac{mn}{(m^2-n^2)^2}\\ 0\end{cases} \tag{5}$$

We were asked to evaluate the matrix elements from the integrals of H_{mn} for when $V(x) = \frac{ax}{L}$. I wrote a function for H_{mn} in Python with inputs n and m which are the dimensions of the matrix and used conditions to solve for the solutions from Equation 1.

$$X = \begin{cases}\frac{\hbar^2\pi^2 n^2}{2ML^2} + \frac{a}{2} & \text{if } m = n\\ \frac{2a}{L^2}(-(\frac{2L}{\pi})^2)\frac{mn}{(m^2-n^2)^2} & \text{if } m \neq n\text{, one even, one odd}\\ 0 & \text{if } m \neq n\text{, both even or odd}\end{cases} \tag{6}$$

I then created an empty matrix and then using a nested for loop with n and m as indices to solve for each element in the matrix by solving the for the value at each position with the H function created earlier. Using this matrix and the eigen functions built into NumPy, I calculated the eigenvalues and eigenvectors for the matrix.

Comparing the results of eigenvalues/allowed energies calculated from a 10 by 10 matrix and a 100 by 100 matrix, I saw little difference in the numbers indicating that even with a 10 by 10 matrix, you can get pretty accurate results.

Lastly, we were asked to calculate the wavefunction in Equation 1 for the ground state and the first two excited states to plot the probability densities of these three states over x (the position of the particle). For this, I created a function with input (x) which essentially used a for loop to sum up entire first row of the matrix of eigenvectors such that ψ_n in Equation 1 was an array of numbers. I did this by indexing the matrix I got from la.eigh with [:,i]. I appended these values into it's own array, which I could then index to get the probability density for individual states. Then I vectorized this function and plotted it over and array for x.

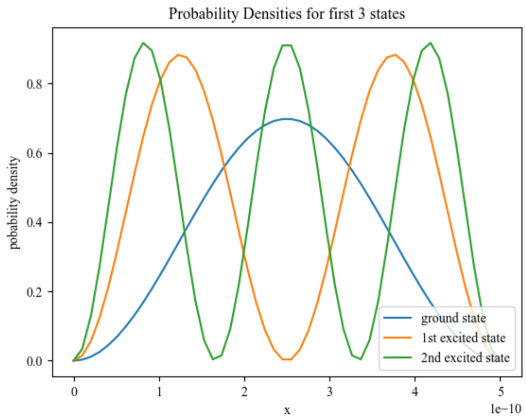


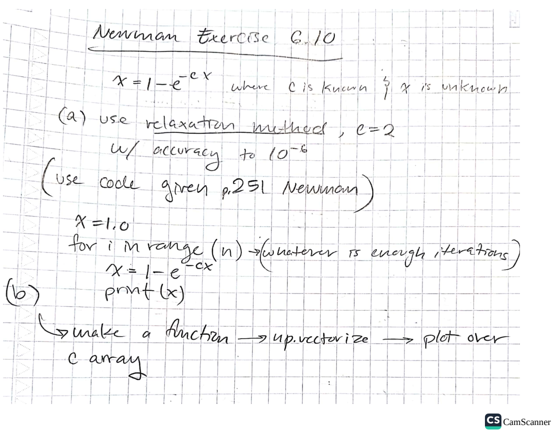
FIG. 5: Wavefunctions over postion.

The result was Figure 5. While the densities do not look very asymmetric, you can clearly see the first three states of the well.

2. EXERCISE 6.10 RELAXATION METHOD

In this exercise, we wrote a program which uses the relaxation method to calculate the solution to Equation 7.

$$x = 1 - e^{-cx} \tag{7}$$



Newman Exercise 6.10

$x = 1 - e^{-cx}$ where c is known & x is unknown

(a) use relaxation method, c=2
w/ accuracy to 10^{-6}
(use code given p.251 Newman)

```
x=1.0
for i in range(n) → (whatever is enough iterations)
    x = 1 - e^{-cx}
    print(x)
```

(b) ↳ make a function → np.vectorize → plot over c array

FIG. 6: Psuedo code for Exercise 6.10.

I then vectorized this program so that I could plot x over an array of c values. I plotted x over c in Figure 7 where there is a clear transition from $x = 0$ to x is a non-zero number as expected. Fortunately, the solution converges to one point and does not oscillate.

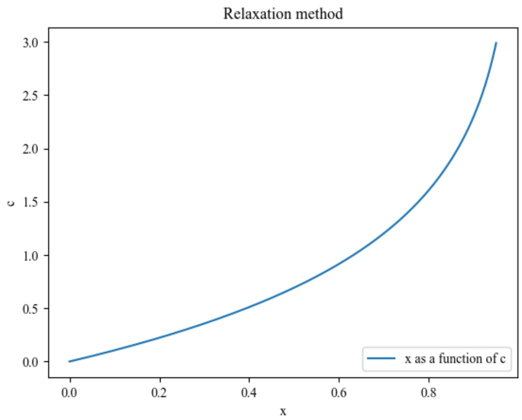


FIG. 7: Plot of x as a function of c.

3. SURVEY QUESTIONS

The homework this week took approximately 9 hours. I found Exercise 6.9 difficult but, overall enjoyed it. Maybe I wish we had more time to work on it. I'm also having troubling fitting the equations on the page in one column and finding a work around.