Computational Physics Final

24100044

Problem 5

part a

Since we now have a discrete set of x values, we can no longer use the derivative operator as one does usually in the Schrodinger equation (SE). We must then find another way to represent and calculate the $\frac{d^2}{dx^2}$ operator. Let us make use of the central difference approach. The second derivative using the central difference is as follows:

$$f'(x) = \frac{f(x + \frac{h}{2} - 2f(x) + f(x + \frac{h}{2})}{h^2} \tag{1}$$

The continuous x in the SE will be replaced by x_j and dx^2 becomes Δx^2, where Δx is a small enough x interval. It is the interval between Let us now apply this to the SE, we get the following:

$$-\left(\frac{\hbar^2}{2m}\frac{\psi(x_{j+1}) - 2\psi(x_j) + \psi(x_{j-1})}{(\Delta x)^2}\right) + V(x_j)\psi(x_j) = E\psi(x_j) \tag{2}$$

We can rearrange this to get the expression given in the question

$$-\left(\psi(x_{j+1}) - 2\psi(x_j) + \psi(x_{j-1})\right) + \frac{2m(\Delta x)^2}{\hbar^2}V(x_j)\psi(x_j) = \frac{2m(\Delta x)^2}{\hbar^2}E\psi(x_j) \tag{3}$$

part b

We first begin by saying that the Hamiltonian can be written in matrix form in the eigenbasis, and as such, its diagonal entries are the energy eigenvalues. I will not be proving this fact as it is rather fundamental. Let us look at the problem at hand. We have the expression

$$-\psi(x_{j+1}) + 2\psi(x_j) - \psi(x_{j-1}) + \frac{2m(\Delta x)^2}{\hbar^2}V(x_j)\psi(x_j) = \frac{2m(\Delta x)^2}{\hbar^2}E\psi(x_j) \tag{4}$$

To begin, the potential and energy values can be redefined to put out of sight the constants attached to them. Then we have

$$-\psi(x_{j+1}) + 2\psi(x_j) - \psi(x_{j-1}) + v(x_j)\psi(x_j) = \epsilon\psi(x_j) \tag{5}$$

If we have normalized states, we can see that the hamiltonian can be represented as

$$(2 + v(x_j)) \tag{6}$$

We put $\psi(x_j)$ as the main diagonal entries of the matrix and we can then immediately see that the diagonals above and below the main diagonal will represent the terms that go with $\psi(x_{j+1})$ and $\psi(x_{j-1})$, respectively. Since we are taking the states to be normalized we can just put them as 1 in the matrix, and since in equation 5, they have a negative sign, the diagonals above and below the main diagonal will be -1.

part e

the boundary conditions are imposed by

Problem 6

Newton's method makes use of the first derivative of the function that we are finding the roots of; it takes the test value of x and draws a tangent at that point.