$$-\psi_{i+1} + (D_i - \lambda)\psi_i - \psi_{i-1} = 0 \qquad , \; i = 1,2,3...\text{n} \qquad (1)$$

Where $D_i = \frac{2m}{\hbar^2}(\Delta x)^2 U_i + 2$, $\lambda = \frac{2m}{\hbar^2}(\Delta x)^2 E$. Δx is the grid step.

Usual boundary conditions are: $\psi_0 = 0$ and $\psi_{n+1} = 0$. Writing (1) for every value of i we gain:

$$\begin{bmatrix} D_1 & -1 & & \\ -1 & D_2 & -1 & \\ & -1 & ..... & -1 \\ & & -1 & D_n \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ ... \\ \psi_n \end{bmatrix} = E \begin{bmatrix} \psi_1 \\ \psi_2 \\ ... \\ \psi_n \end{bmatrix} \qquad (2)$$

Eq. (2) represents an eigenvalue problem, with mentioned boundary conditions, which can easily be solved.

Now, if we are working with a symmetric potential, wavefunctions could be either even or odd. When I just restrict domain of the problem with condition x>0 , Eq. (2) yields only odd solutions, since the written boundary conditions correspond to this problem (odd wavefunction crosses zero in x=0.

Even parity wavefunctions require different boundary condition in x=0. Let's say $\psi_0 = M$, where M is some constant that will be changed during the normalisation process. For me, now the problem is the formulation of the equation that is similar to Eq.(2).

For i=1: $-\psi_2 + (D_1 - \lambda)\psi_1 - M = 0$, and all the other equations are the same as in the previous formulation. It seems to me that one way of writing this system is like this:

$$\begin{bmatrix} D_1 & -1 & & \\ -1 & D_2 & -1 & \\ & -1 & ..... & -1 \\ & & -1 & D_n \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ ... \\ \psi_n \end{bmatrix} = E \begin{bmatrix} \psi_1 \\ \psi_2 \\ ... \\ \psi_n \end{bmatrix} + \begin{bmatrix} M \\ 0 \\ ... \\ 0 \end{bmatrix} \qquad (2)$$

What looks like even more complicated than ordinary eigenvalue problem, and I have no idea how to solve it from here. Probably parameter M should be taken into account in a different way.