

PX390

Abubakar Omar

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1 Introduction

$$\begin{aligned} -\frac{\partial^2}{\partial x^2}\Psi(x) + P(x)\Psi(x) &= E\Psi(x) \\ -\frac{(\Psi_{i-1} - 2\Psi_i + \Psi_{i+1}))}{(\Delta x)^2} + P_i\Psi_i &= E\Psi_i \\ \frac{-(\Psi_{i-1} - 2\Psi_i + \Psi_{i+1})) + (\Delta x)^2 P_i\Psi_i}{(\Delta x)^2} &= E\Psi_i \\ \frac{-\Psi_{i-1} + 2\Psi_i - \Psi_{i+1} + (\Delta x)^2 P_i\Psi_i}{(\Delta x)^2} &= E\Psi_i \\ \frac{-\Psi_{i-1} + (2 + (\Delta x)^2 P_i)\Psi_i - \Psi_{i+1}}{(\Delta x)^2} &= E\Psi_i \\ \frac{1}{(\Delta x)^2}(-\Psi_{i-1} + (2 + (\Delta x)^2 P_i)\Psi_i - \Psi_{i+1}) &= E\Psi_i \end{aligned} \tag{1}$$
$$i = 1, 2, 3, \dots, N - 2$$

2 Boundary condition 1

$$\begin{aligned} a_L\Psi(x_L) + b_L\Psi'(x_L) &= 0 \\ a_L\Psi_0 + b_L\Psi'_0 &= 0 \\ a_L\Psi_0 + b_L\left(\frac{\Psi_1 - \Psi_{-1}}{2\Delta x}\right) &= 0 \\ 2a_L\Delta x\Psi_0 + b_L(\Psi_1 - \Psi_{-1}) &= 0 \\ 2a_L\Delta x\Psi_0 + b_L\Psi_1 - b_L\Psi_{-1} &= 0 \\ 2a_L\Delta x\Psi_0 + b_L\Psi_1 &= b_L\Psi_{-1} \\ \frac{2a_L\Delta x}{b_L}\Psi_0 + \Psi_1 &= \Psi_{-1} \\ \Psi_{-1} &= \frac{2a_L\Delta x}{b_L}\Psi_0 + \Psi_1 \end{aligned} \tag{2}$$

Substituting $i = 0$ into (1) gives:

$$\frac{1}{(\Delta x)^2}(-\Psi_{-1} + (2 + (\Delta x)^2 P_0)\Psi_0 - \Psi_1) = E\Psi_0 \quad (3)$$

Now substitute (1) into (3):

$$\begin{aligned} \frac{1}{(\Delta x)^2} \left(\left(-\frac{2a_L \Delta x}{b_L} \Psi_0 - \Psi_1 \right) + (2 + (\Delta x)^2 P_0)\Psi_0 - \Psi_1 \right) &= E\Psi_0 \\ \frac{1}{(\Delta x)^2} \left(-\frac{2a_L \Delta x}{b_L} \Psi_0 + (2 + (\Delta x)^2 P_0)\Psi_0 - 2\Psi_1 \right) &= E\Psi_0 \\ \frac{1}{(\Delta x)^2} \left(\left(-\frac{2a_L \Delta x}{b_L} + (2 + (\Delta x)^2 P_0) \right) \Psi_0 - 2\Psi_1 \right) &= E\Psi_0 \end{aligned} \quad (4)$$

3 Boundary condition 2

$$a_R \Psi(x_R) + b_R \Psi'(x_R) = 0$$

$$\begin{aligned} a_R \Psi_{N-1} + b_R \Psi'_{N-1} &= 0 \\ a_R \Psi_{N-1} + b_R \left(\frac{\Psi_N - \Psi_{N-2}}{2\Delta x} \right) &= 0 \\ 2a_R \Delta x \Psi_{N-1} + b_R (\Psi_N - \Psi_{N-2}) &= 0 \\ 2a_R \Delta x \Psi_{N-1} + b_R \Psi_N - b_R \Psi_{N-2} &= 0 \\ b_R \Psi_N &= b_R \Psi_{N-2} - 2a_R \Delta x \Psi_{N-1} \\ \Psi_N &= \Psi_{N-2} - \frac{2a_R \Delta x}{b_R} \Psi_{N-1} \end{aligned} \quad (5)$$

Substituting $i = N - 1$ into (1) gives:

$$\frac{1}{(\Delta x)^2}(-\Psi_{N-2} + (2 + (\Delta x)^2 P_{N-1})\Psi_{N-1} - \Psi_N) = E\Psi_{N-1} \quad (6)$$

Now substitute (5) into (6):

$$\begin{aligned} \frac{1}{(\Delta x)^2} \left(-\Psi_{N-2} + (2 + (\Delta x)^2 P_{N-1})\Psi_{N-1} - \left(\Psi_{N-2} - \frac{2a_R \Delta x}{b_R} \Psi_{N-1} \right) \right) &= E\Psi_{N-1} \\ \frac{1}{(\Delta x)^2} \left(-2\Psi_{N-2} + (2 + (\Delta x)^2 P_{N-1})\Psi_{N-1} + \frac{2a_R \Delta x}{b_R} \Psi_{N-1} \right) &= E\Psi_{N-1} \\ \frac{1}{(\Delta x)^2} \left(-2\Psi_{N-2} + \left((2 + (\Delta x)^2 P_{N-1}) + \frac{2a_R \Delta x}{b_R} \right) \Psi_{N-1} \right) &= E\Psi_{N-1} \\ \frac{1}{(\Delta x)^2} \left(-2\Psi_{N-2} + \left((2 + (\Delta x)^2 P_{N-1}) + \frac{2a_R \Delta x}{b_R} \right) \Psi_{N-1} \right) &= E\Psi_{N-1} \end{aligned} \quad (7)$$

4 Matrix

Putting everything together we have:

$$\frac{1}{(\Delta x)^2} \begin{pmatrix} -\frac{2a_L \Delta x}{b_L} + (2 + (\Delta x)^2 P_0) & -2 & & & \\ -1 & (2 + (\Delta x)^2 P_1) & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & (2 + (\Delta x)^2 P_{N-2}) & -1 \\ & & & -2 & (2 + (\Delta x)^2 P_{N-1}) + \frac{2a_R \Delta x}{b_R} \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{N-2} \\ \psi_{N-1} \end{pmatrix} = E \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{N-2} \\ \psi_{N-1} \end{pmatrix}$$

(4) and (7) correspond to the first and last row of the matrix respectively and the rest of the matrix is filled using (1)

$$M\Psi = E\Psi$$

Then iterate:

$$\Psi_{i+1} = (M - E_0 I)^{-1} \Psi_i$$

[By choosing an initial guess for Ψ_0]