PX390

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1 Introduction

$$-\frac{\partial^2}{\partial x^2}\Psi(x) + P(x)\Psi(x) = E\Psi(x)$$

$$\begin{aligned}
-\frac{(\Psi_{i-1} - 2\Psi_i + \Psi_{i+1})}{(\Delta x)^2} + P_i\Psi_i &= E\Psi_i \\
\frac{-(\Psi_{i-1} - 2\Psi_i + \Psi_{i+1}) + (\Delta x)^2 P_i\Psi_i}{(\Delta x)^2} &= E\Psi_i \\
\frac{-\Psi_{i-1} + 2\Psi_i - \Psi_{i+1} + (\Delta x)^2 P_i\Psi_i}{(\Delta x)^2} &= E\Psi_i \\
\frac{-\Psi_{i-1} + (2 + (\Delta x)^2 P_i)\Psi_i - \Psi_{i+1}}{(\Delta x)^2} &= E\Psi_i
\end{aligned}$$

$$\frac{1}{(\Delta x)^2}(-\Psi_{i-1} + (2 + (\Delta x)^2 P_i)\Psi_i - \Psi_{i+1}) = E\Psi_i \tag{1}$$

$$i = 1, 2, 3, \ldots, N-2$$

2 Boundary condition 1

$$a_L\Psi(x_L) + b_L\Psi'(x_L) = 0$$

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

$$\Psi_{-1} = \frac{2a_L\Delta x}{b_L}\Psi_0 + \Psi_1 \tag{2}$$

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

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

Now substitute (1) into (3):

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

3 Boundary condition 2

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

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

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

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

Now substitute (5) into (6):

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

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

4 Matrix

Putting everything together we have:

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

(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]