

1 Boundary Conditions

Starting from TISE, we will impose two types of boundary conditions.

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + -\sum_{n=0}^N \alpha(x-x_n) \delta_x \psi = E\psi$$

$$\psi(x) = \begin{cases} A_n e^{ikx} + B_n e^{-ikx}, & x_{n-1} < x < x_n \\ A_{n+1} e^{ikx} + B_{n+1} e^{-ikx}, & x_n < x < x_{n+1} \end{cases}$$

We will first impose the continuity of the wave function, by:

$$\psi_+(x_n) = \psi_-(x_n)$$

$$A_n e^{ikx} + B_n e^{-ikx} = A_{n+1} e^{ikx} + B_{n+1} e^{-ikx}$$

Then, we will solve Schrodinger's equations to see the other relation we can use as a boundary condition:

$$\psi''(x) = -\frac{2m\psi(x)E - \alpha\delta_x(x-x_n)}{\hbar^2}$$

$$\int_{x_n-\epsilon}^{x_n+\epsilon} \psi''(x)dx = \int_{x_n-\epsilon}^{x_n+\epsilon} -\frac{2m\psi(x)E - \alpha\delta_x(x-x_n)}{\hbar^2} dx$$

$$\psi'(x_n + \epsilon) - \psi'(x_n - \epsilon) = \frac{2\alpha m\psi(x_n)}{\hbar^2}$$

$$\lim_{\epsilon \rightarrow 0} (\psi'(x_n + \epsilon) - \psi'(x_n - \epsilon)) = \psi'_+(x_n) - \psi'_-(x_n)$$

$$\psi'_+(x_n) - \psi'_-(x_n) = \frac{2\alpha m\psi(x_n)}{\hbar^2}$$

$$ikA_n e^{ikx_n} - ikB_n e^{-ikx_n} = ikA_{n+1} e^{ikx_n} - ikB_{n+1} e^{-ikx_n} = \frac{2\alpha m (A_n e^{ikx_n} + B_n e^{-ikx_n})}{\hbar^2}$$

Introducing $\beta = \frac{\alpha m}{\hbar^2}$. Then simplifying the second boundary condition:

$$ikA_{n+1} e^{ikx_n} + -ikA_n e^{ikx_n} - ikB_{n+1} e^{-ikx_n} + ikB_n e^{-ikx_n} = \frac{2\alpha m (A_n e^{ikx_n} + B_n e^{-ikx_n})}{\hbar^2}$$

$$e^{-ikx_n} (-A_n e^{2ikx_n} + B_n + A_{n+1} e^{2ikx_n} - B_{n+1}) = -\frac{2i\alpha m (A_n e^{ikx_n} + B_n e^{-ikx_n})}{k\hbar^2}$$

$$-A_n e^{2ikx_n} + B_n + A_{n+1} e^{2ikx_n} - B_{n+1} = -2i\beta (A_n e^{2ikx_n} + B_n)$$

2 Deriving The Matrix M_n

Now we will write a matrix of this form:

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = M_n \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

Using our two boundary conditions (1) & (2)

$$A_n e^{ikx} + B_n e^{-ikx} = A_{n+1} e^{ikx} + B_{n+1} e^{-ikx} \quad (1)$$

$$-A_n e^{2ikx_n} + B_n + A_{n+1} e^{2ikx_n} - B_{n+1} = -2i\beta (A_n e^{2ikx_n} + B_n) \quad (2)$$

The resultant matrix will be:

$$A_{n+1} = -i (A_n \beta + i A_n + \beta B_n e^{-2ikx_n})$$

$$B_{n+1} = i A_n \beta e^{2ikx_n} + i \beta B_n + B_n$$

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \begin{pmatrix} 1 - i\beta & -i\beta e^{-2ikx_n} \\ i\beta e^{2ikx_n} & 1 + i\beta \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

Setting $n = 0, 1, 2$. The results will be:

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M_0 \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} \quad \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = M_1 \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \quad \begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = M_2 \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

Back substitution yields:

$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = M_2 M_1 M_0 \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}$$

Thus, The matrix M_n is going to be this:

$$\begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix} = \prod_{n=0}^N M_n \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}$$

3 Computing T

Using the boundary conditions (1)&(2), and setting $B_{N+1} = 0$, we will obtain this:

$$A_{N+1} = -i (A_0\beta + iA_0 + \beta B_0 e^{-2ikx_0}) \quad (3)$$

$$B_{N+1} = iA_0\beta e^{2ikx_0} + i\beta B_0 + B_0 \quad (4)$$

$$A_0\beta e^{2ikx_0} + (\beta - i)B_0 = 0$$

$$A_0 \rightarrow \frac{iB_0 e^{-2ikx_0} - \beta B_0 e^{-2ikx_0}}{\beta} \quad (5)$$

Substituting (5) in (3) then dividing by A_0 yields the transmission coefficient T:

$$T = \left| \frac{A_{N+1}}{A_0} \right|^2 = \frac{1}{\beta^2 + 1} = \frac{1}{|M_{22}|^2}$$

3.1 Bonus: Checking R + T = 1

We will first compute R, then we will add it to T and we expect the results to be 1. This is done by substituting (5) in (4) then dividing by A_0 , which will yield the following:

$$R = \left| \frac{B_{N+1}}{A_0} \right|^2 = \frac{\beta^2}{\beta^2 + 1}$$

Then,

$$T + R = \frac{1}{\beta^2 + 1} + \frac{\beta^2}{\beta^2 + 1} = 1$$

4 Numerical Work

Now we will numerically compute the transmission coefficient T as a function of k while setting other constants to 1. The detailed approach is present in the Mathematica file, after doing so. We will get these nice plots:

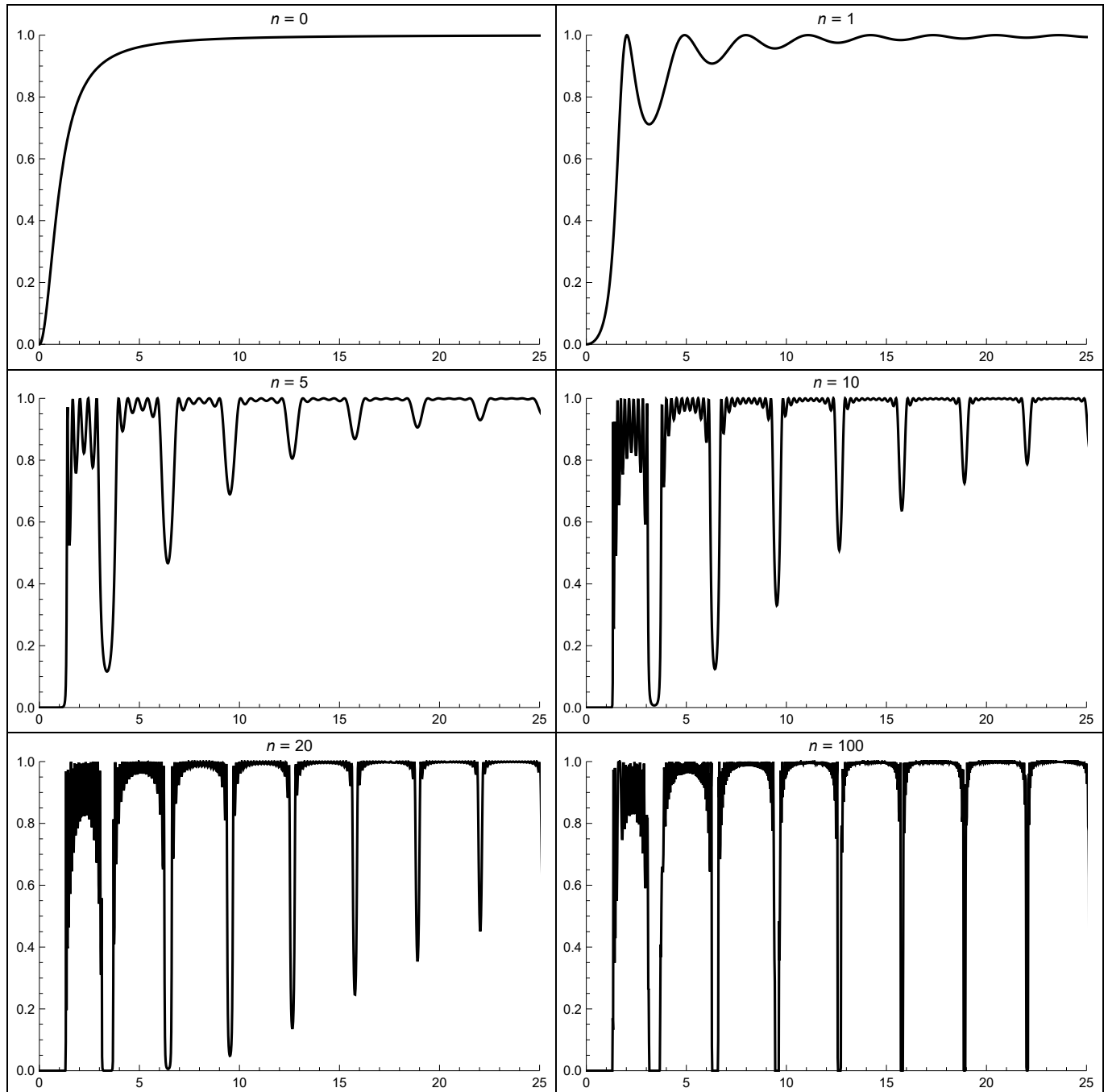


Figure 1. T vs k , we can see the allowed energy zones when $T \approx 1$, and band gaps when $T \approx 0$. a, m, \hbar and α are set equal to 1.

4.1 T Versus N Delta Potential

Here, I was unable to generate this plot myself nor was I able to find the relation. I will cite professor Griffith's formula then I will plot it using Mathematica.

$$T(n) = \frac{1}{1 - [\beta U_n(z)]^2}$$

Where $U_n(z)$ is the second type of Chebyshev polynomials and z is $(-1)^n$

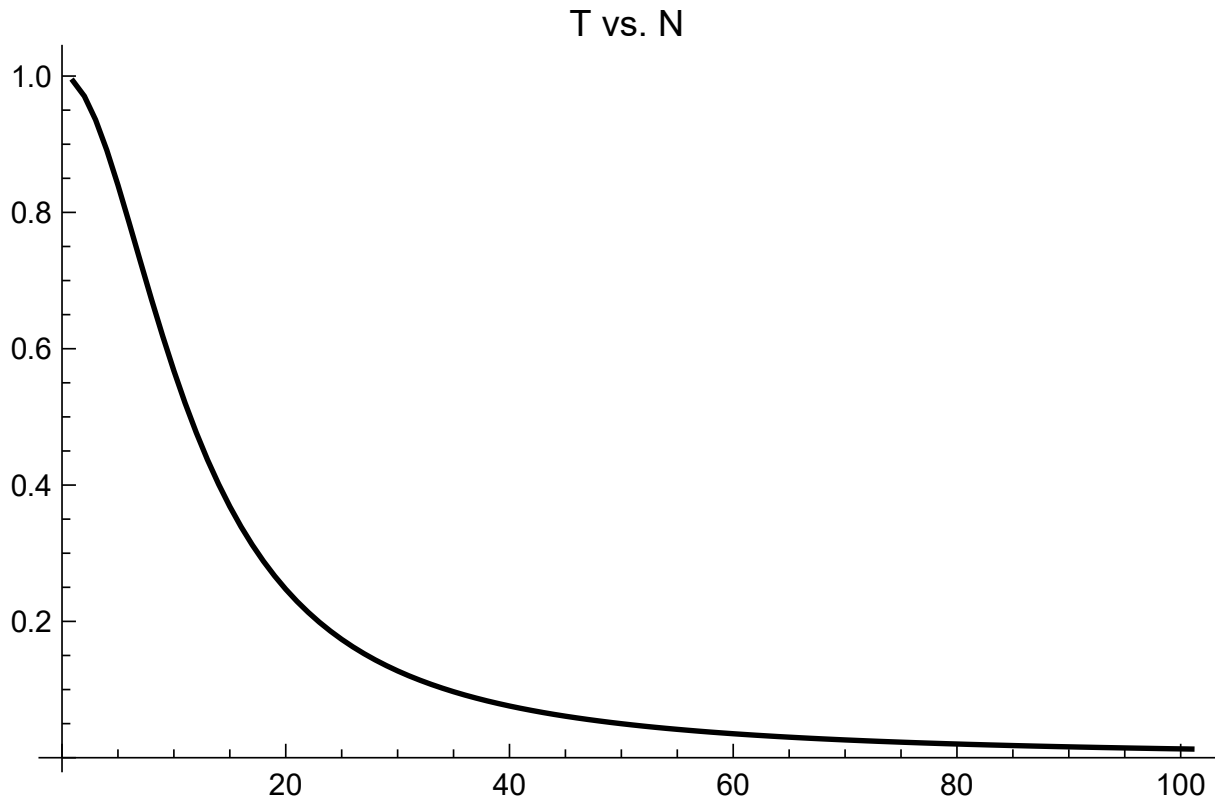


Figure 2. T vs N, The plot of $T(n)$ where k is set to be 36