1 Boundary Conditions

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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)

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

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

The resultant matrix will be:

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

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

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

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

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

Back subsitution 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:

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

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

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

$$A_0 \to \frac{iB_0 e^{-2ikx_0} - \beta B_0 e^{-2ikx_0}}{\beta} \tag{5}$$

Subsituting (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 subsituting (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,

$$T + R = \frac{1}{\beta^2 + 1} + \frac{\beta^2}{\beta^2 + 1} = 0$$

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:

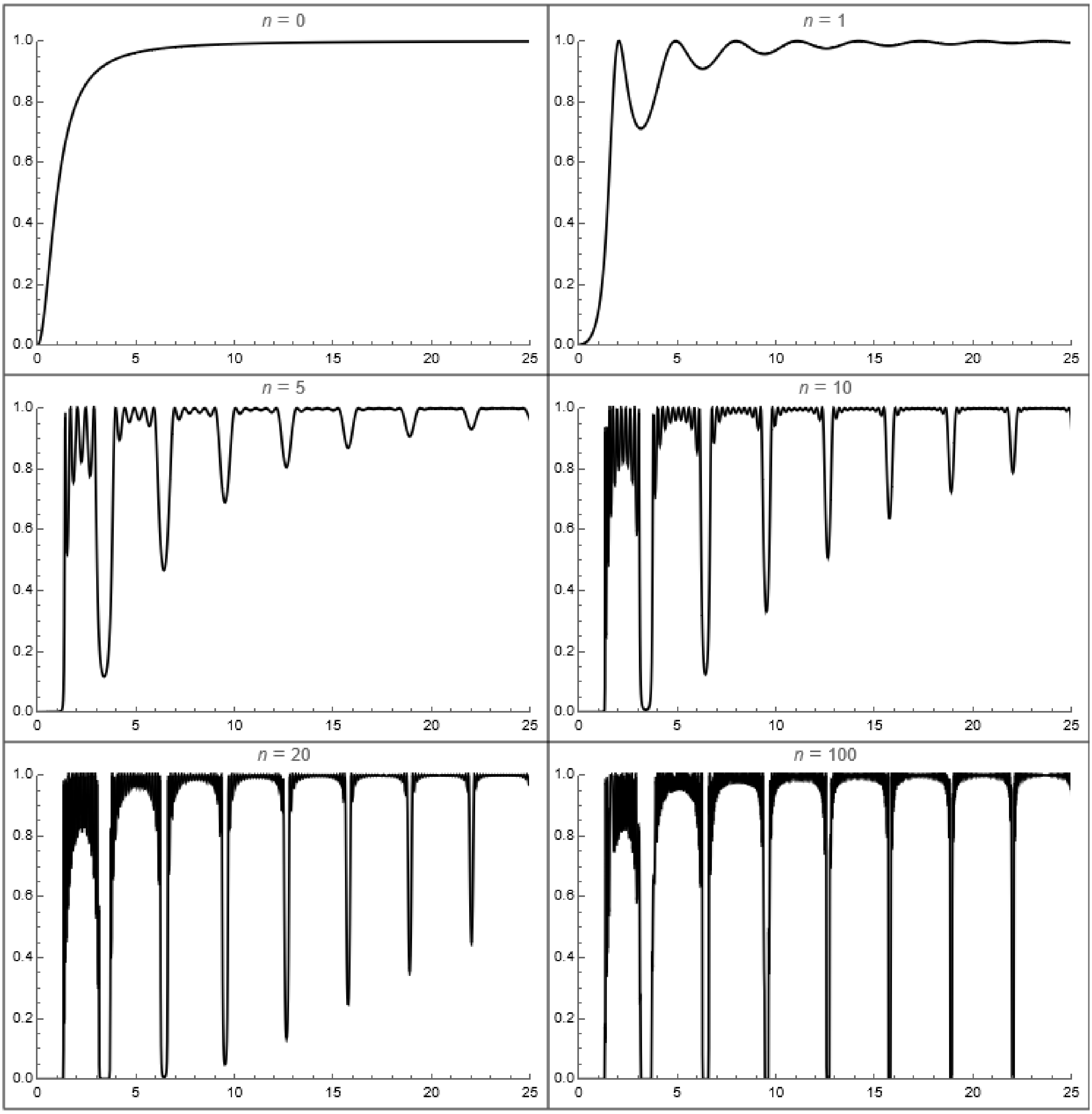

Figure 1. T vs k, we can see the allowed energy zones when T $\approx$ 1, and band gaps when T $\approx$ 0. a, m, $\hbar$ and α are set equal to 1.

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 $(-1)^n$

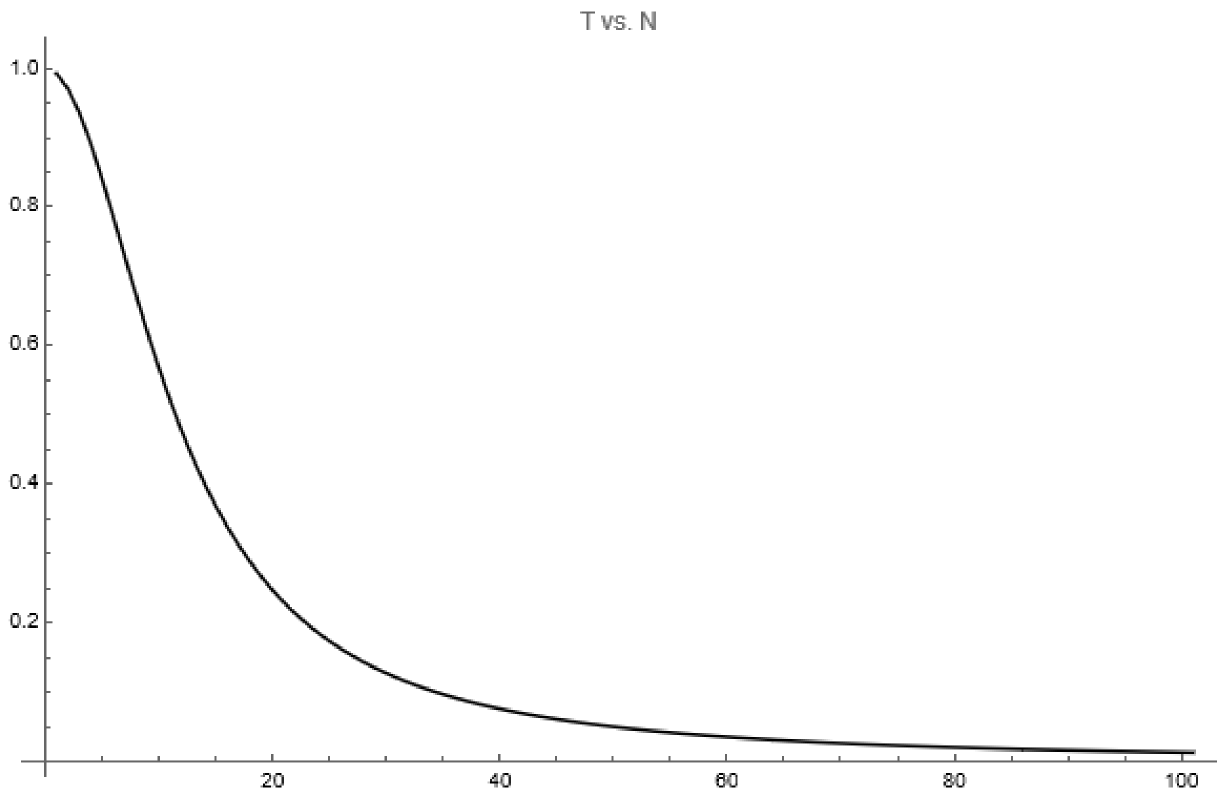

Figure 2. T vs N, The plot of T(n) where k is set to be 36