1 Problem Set Up

The main objective of this homework is to construct the transfer matrix M, and use it to solve two types of quantum potentials.

1.1 The Main Approach

The first thing we want to do is to discretize our potential function, in the same fashion as approximating the area of a function through a series of rectangles with a width Δx.

Our potential has the following form:

$$V_{\pm}(x) = \pm \frac{\hbar^2}{2a^2 m} \frac{n(n+1)}{\cosh^2(x/a)}$$

For the purpose of this numerical approach, I set $a = \hbar = m = n = 1$.

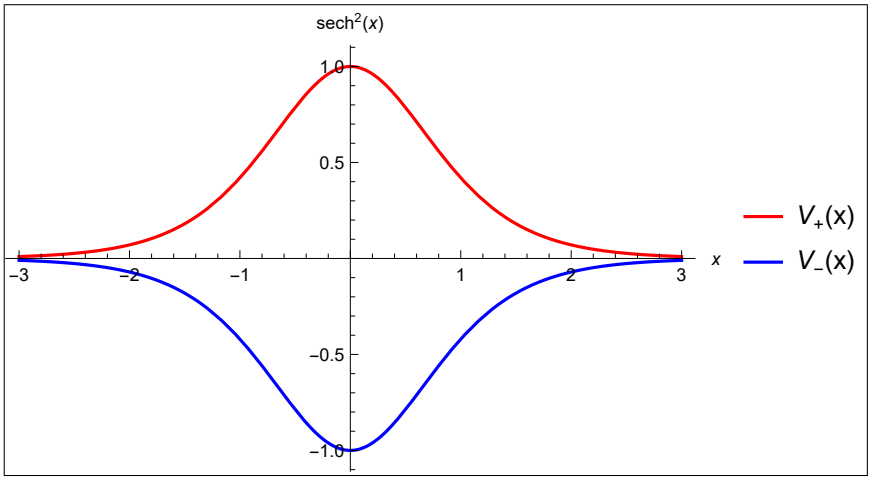

Figure 1: $V_{\pm}(x)$

Now, I will split $V_+(x)$ into rectangles with $\Delta x = 0.5$:

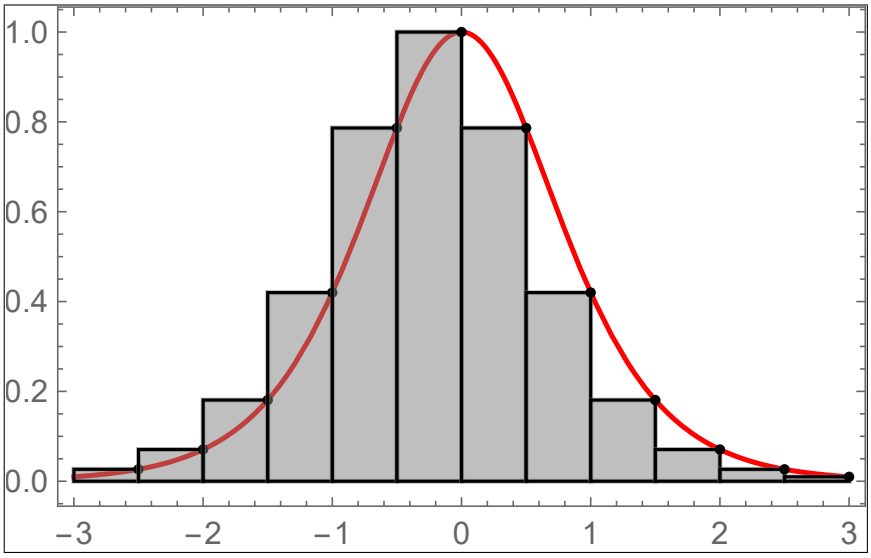

Figure 2: Discretized $V_+(x)$ with $\Delta x = 0.5$, and points taken from the right

Now that we Discretized $V_{\pm}(x)$, we can return to physics and start examining the new potential from Schrodinger's equation point of view.

1.2 Recognizing Regions

Now, we will have two types of regions to deal with: **Constant Potential** and **Step Potential**. Each one of them will produce one type of transfer matrix, and the overall transfer matrix is just the multiplication of these matrices.

$$V \approx V_0 + V_1 + \cdots + V_N$$

1.2.1 Constant Potential

For a constant potential, the solution of Schrodinger's equation is known, which is:

$$\psi(x) = Ae^{ik_n x} + Be^{-ik_n x}; \qquad k_n = \sqrt{2(E - V_n)}$$

Now, we need to find the transfer matrix M_0 that will transfer the wavefunction from the beginning of the potential x_i to the end of it x_f, with $dx = x_f - x_i$:

$$\psi_i = \begin{bmatrix} Ae^{ik_n x_i} \\ Be^{-ik_n x_i} \end{bmatrix}, \quad \psi_f = \begin{bmatrix} Ae^{ik_n x_f} \\ Be^{-ik_n x_f} \end{bmatrix}$$

We can see that each component of ψ_f is $\pm e^{ik_n(x_f - x_i)} = \pm e^{ik_n dx}$. We can write a transfer matrix with this shift as:

$$\psi_f = \begin{bmatrix} e^{ik_n dx} & 0 \\ 0 & e^{-ik_n dx} \end{bmatrix} \psi_i$$

Since dx is constant across all constant potentials, and the only changing factor is k:

$$\therefore M_c(k_n) = \begin{bmatrix} e^{ik_n dx} & 0 \\ 0 & e^{-ik_n dx} \end{bmatrix}$$

1.2.2 Step Potential

For the step potential, we will need to use the boundary condition of the wavefunction, namely the continuity of the wavefunction, and the continuity of its derivative. Between two infinitesimal points around the boundary x_{0-} and x_{0+}:

$$\psi(x_{0-}) = \psi(x_{0+})$$

$$\psi_+(x_{0-}) + \psi_-(x_{0-}) = \psi_+(x_{0+}) + \psi_-(x_{0+}) \tag{1}$$

and

$$\psi'(x_{0-}) = \psi'(x_{0+})$$

$$k_n\left[\psi_+(x_{0-})-\psi_-(x_{0-})\right]=k_{n+1}\left[\psi_+(x_{0+})-\psi_-(x_{0+})\right] \tag{2}$$

Combining (1) & (2) in matrices yield:

$$\begin{bmatrix}1 & 1\\ k_n & -k_n\end{bmatrix}\begin{bmatrix}\psi_+(x_{0-})\\ \psi_-(x_{0-})\end{bmatrix}=\begin{bmatrix}1 & 1\\ k_{n+1} & -k_{n+1}\end{bmatrix}\begin{bmatrix}\psi_+(x_{0+})\\ \psi_-(x_{0+})\end{bmatrix}$$

$$\begin{bmatrix}\psi_+(x_{0+})\\ \psi_-(x_{0+})\end{bmatrix}=\frac{1}{2}\begin{bmatrix}1+\frac{k_n}{k_{n+1}} & 1-\frac{k_n}{k_{n+1}}\\ 1-\frac{k_n}{k_{n+1}} & 1+\frac{k_n}{k_{n+1}}\end{bmatrix}\begin{bmatrix}\psi_+(x_{0-})\\ \psi_-(x_{0-})\end{bmatrix}$$

$$\therefore M_s(k_n,k_n+1)=\begin{bmatrix}1+\frac{k_n}{k_{n+1}} & 1-\frac{k_n}{k_{n+1}}\\ 1-\frac{k_n}{k_{n+1}} & 1+\frac{k_n}{k_{n+1}}\end{bmatrix}$$

1.3 Finalization

Now that we obtained an expression for M_c and M_s, we can now use them consecutively to transfer the wavefunction from the leftmost position of the potential to the rightmost. From the incident wavefunction Ψ_I to the transmitted one Ψ_T.

$$\Psi_T=M_s(k_{N-1},k_N)M_c(k_{N-1})\dots M_c(k_1)M_s(k_0,k_1)\Psi_I$$

$$\Psi_T=\mathbf{M}(k_n,k_{n+1})\Psi_I$$

$$\mathbf{M}(k_n,k_{n+1})=\left(\prod_{n=0}^{N-1}\left(M_s(k_n,k_{n+1})M_c(k_{n+1})\right)^T\right)^T$$

The usage of transpose in $\left(\prod_{n=0}^{N-1}x_n^T\right)^T$ is to ensures that the product is taken in the inverse order, starting from n=N-1 to n=0.

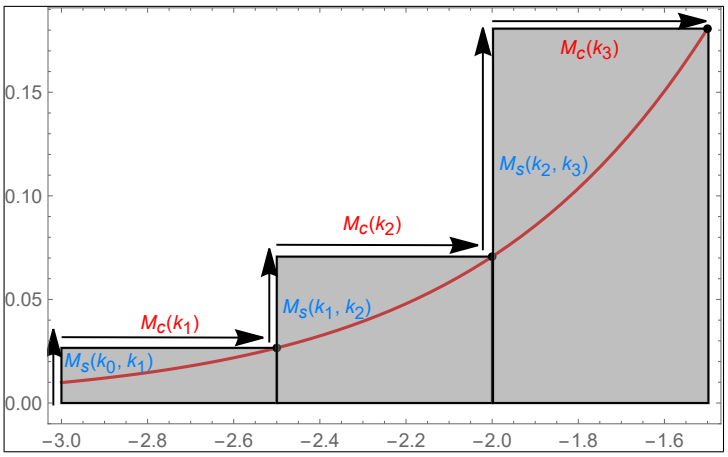

Figure 3: Snippet of the series of transfer matrices that will take us from Ψ_I to Ψ_T

2 Numerical Calculations

Using Mathematica, with this code:

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V[x_, q_, n_] := q n (n + 1) / (2 Cosh[x]^2)

k[x_, q_, n_] := Sqrt[2 (En - V[x, q, n])]

Mc[x_, q_, n_, dx_] := {{E^(I k[x,q,n]*dx), 0}, {0, E^(-I k[x,q,n]*dx)}}

Ms[x_, q_, n_, dx_] := 0.5 * {{1 + k[x, q, n]/k[x + dx, q, n], 1 - k[x, q, n]/k[x + dx, q, n]}, {1 - k[x, q, n]/k[x + dx, q, n], 1 + k[x, q, n]/k[x + dx, q, n]}}

listmultiplier[list_, partitionwidth_ : 5] :=
 NestWhile[Dot @@@ Partition[#, partitionwidth, partitionwidth, 1, {}] &, list, Dimensions[#][[1]] > 1 &][[1]]

BigM[q_, n_, dx_] := Reverse@Table[Ms[x, q, n, dx].Mc[x, q, n, dx], {x, -3, 3, dx}] // N;

Mlist1 = BigM[1, 1, 0.005]; Mlist2 = BigM[-1, 1, 0.005];

Plot[{1/(ComplexExpand@Abs@listmultiplier[Mlist1, 10][[2]][[2]])^2, 1/(ComplexExpand@Abs@listmultiplier[Mlist2, 10][[2]][[2]])^2},
 {En, 0, 1}, PlotRange -> All, PlotStyle -> {Black, Red}, PlotLegends -> {"T∈V+", "T∈V-"}, AxesLabel -> {"E", "T"},
 PlotLabel -> "T(E), for n = 1"]
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Figure 4: Mathematica implementation of the transfer matrix approach

I obtained this result:

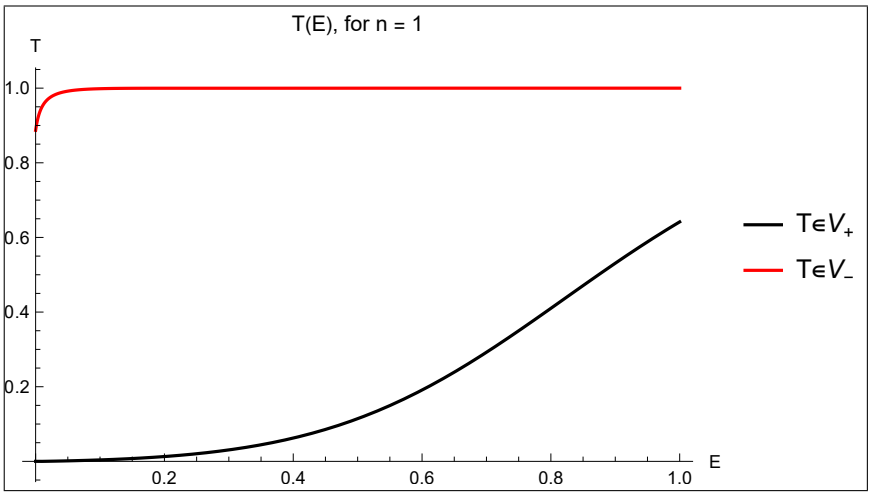

Figure 5: Transmission coefficient as a function of energy, $\Delta x = 0.005$, which means I have split the potential into 1200 rectangle