Note on transmission and reflection coefficients.

1 Problem setup

As shown in Figure 1, consider the piecewise linear potential function $V(x)$:

$$\begin{aligned} V(x) &= s_j(x - x_j) + V_j, \\ s_j &= (V_{j+1/2} - V_{j-1/2})/\Delta x, \\ V_j &= (V_{j+1/2} + V_{j-1/2})/2, \end{aligned} \tag{1}$$

where $j = 0, 1, 2, \cdots, N$ for $x_{j-1/2} < x < x_{j+1/2}$. test

Take a quantum barrier in the interval $\mathcal{Q} = [x_j, x_{j+1}]$ and take the potential to be constant outside this barrier $V(x) = V_j$ in $\mathcal{C}_j = (-\infty, x_j)$ and $V(x) = V_{j+1}$ in $\mathcal{C}_{j+1} = (x_{j+1}, \infty)$. For a state $E = p^2/2m$ the time-independent Schrödinger equation

$$-\varepsilon^2 \psi''(x) + 2mV(x)\psi(x) = p^2\psi(x) \tag{2}$$

has the solution

$$\psi(x) = \begin{cases} a_1 e^{i\kappa_j (x - x_j)/\varepsilon} + b_1 e^{-i\kappa_j (x-x_j)/\varepsilon}, & x \in \mathcal{C}_j \\ \psi_{\mathcal{Q}}, & x \in \mathcal{Q} \\ a_2 e^{i\kappa_{j+1}(x - x_{j+1})/\varepsilon} + b_2 e^{-i\kappa_{j+1}(x - x_{j+1})/\varepsilon}, & x \in \mathcal{C}_{j+1} \end{cases} \tag{3}$$

where $\kappa_{j,j+1} = \sqrt{p^2 - 2mV_{j,j+1}}$ and the coefficients a_1, b_1, a_2 and b_2 are uniquely determined by the boundary conditions at x_1 and x_2. $\psi_{\mathcal{Q}}$ can be determined using the boundary conditions at $x_j, x_{j+1/2}$ and x_{j+1} according to the paper you mention. Hence, for each momentum p we may relate the solution in $\mathcal{C}_{j+1}$ with the solution $\mathcal{C}_j$ in terms of the transfer matrix M

$$\begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = M \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix}. \tag{4}$$

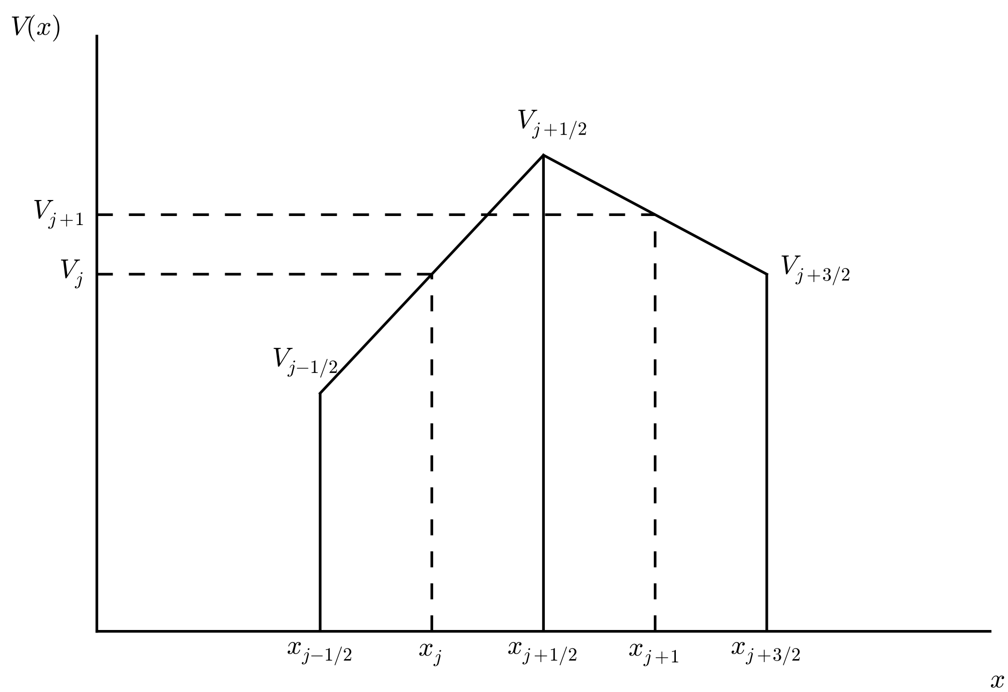

Figure 1: The showcase of the problem.

One may also express the solutions in $\mathcal{C}_j$ and $\mathcal{C}_{j+1}$ in terms of a scattering matrix S which relates the incident and scattered waves

$$\begin{pmatrix} b_1 \\ a_2 \end{pmatrix} = S \begin{pmatrix} a_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} r_1 & t_2 \\ t_1 & r_2 \end{pmatrix} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} -m_{21}/m_{22} & 1/m_{22} \\ \Delta/m_{22} & m_{12}/m22 \end{pmatrix} \begin{pmatrix} a_1 \\ b_2 \end{pmatrix} \tag{5}$$

where $\Delta = \det M = m_{11}m_{22} - m_{12}m_{21}$. By considering the time evolution of the position density $\rho(x,t) = |\psi(x,t)|^2$ in the Schrödinger equation, one derives the continuity equation

$$\frac{\partial}{\partial t}\rho + \nabla \cdot J = 0, \tag{6}$$

where the current density $J(x) = \varepsilon m^{-1} \mathrm{Im}(\bar{\psi}\nabla\psi)$. From (3) one has that

$$J(x) = \begin{cases} \kappa_j(|a_1|^2 - |b_1|^2)/m, & x \in \mathcal{C}_j \\ \kappa_{j+1}(|a_2|^2 - |b_2|^2)/m, & x \in \mathcal{C}_{j+1} \end{cases} \tag{7}$$

so for a wave incident on the barrier from the left ($b_2 \equiv 0$), we have $a_2 = t_1 a_1$ and $b_1 = r_1 a_1$. It follows that the reflection coefficient R_1, the ratio of the reflected to incident current densities, and the transmission coefficient T_1, the ratio of the transmitted to incident current densities, are

$$R_1 = |r_1|^2 \quad \text{and} \quad T_1 = (\kappa_{j+1}/\kappa_j)|t_1|^2. \tag{8}$$

Similarly, for a wave incident from the right

$$R_2 = |r_2|^2 \quad \text{and} \quad T_2 = (\kappa_j/\kappa_{j+1})|t_2|^2. \tag{9}$$

For conclusion, if we have the transfer matrix M as in (4), then by using (5) we can get S. Finally, using (8) or (9) we can get the transmission and reflection coefficients.

2 Calculation of M

Let us find the form of M. So first we will solve the equation (2) in the interval $\mathcal{Q} = [x_j, x_{j+1}]$. Notice on the half interval $[x_j, x_{j+1/2}]$, equation (2) reads:

$$-\varepsilon^2\psi''(x) + [2m(s_j(x - x_j) + V_j) - p^2]\psi(x) = 0, \quad x \in [x_j, x_{j+1/2}]. \tag{10}$$

If we apply a change of variable to x:

$$z_j(x) = \sqrt[3]{\frac{2ms_j}{\varepsilon^2}}(x - b_j), \quad x \in [x_j, x_{j+1/2}] \tag{11}$$

where $b_j = x_j + p^2/2ms_j - V_j/s_j$. Then the equation (10)) changes to

$$\psi''(z_j) - z_j\psi(z_j) = 0 \tag{12}$$

which is the standard Airy equation. The solution of this equation is the airy function:

$$\psi_{\mathcal{Q}}(z_j(x)) = C_j^{(1)}\mathrm{Ai}(z_j(x)) + C_j^{(2)}\mathrm{Bi}(z_j(x)). \tag{13}$$

To determine the coefficients, notice the continuity of ψ and its derivative ψ' at x_j:

$$\begin{pmatrix} 1 & 1 \\ i\kappa_j/\varepsilon & -i\kappa_j/\varepsilon \end{pmatrix}\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} \mathrm{Ai}(z_j(x_j)) & \mathrm{Bi}(z_j(x_j)) \\ \sqrt[3]{\frac{2ms_j}{\varepsilon^2}}\mathrm{Ai}'(z_j(x_j)) & \sqrt[3]{\frac{2ms_j}{\varepsilon^2}}\mathrm{Bi}'(z_j(x_j)) \end{pmatrix}\begin{pmatrix} C_j^{(1)} \\ C_j^{(2)} \end{pmatrix}. \tag{14}$$

For convenience, we wil denote:

$$M_j(x) \equiv \begin{pmatrix} \mathrm{Ai}(z_j(x)) & \mathrm{Bi}(z_j(x)) \\ \sqrt[3]{\frac{2ms_j}{\varepsilon^2}}\mathrm{Ai}'(z_j(x)) & \sqrt[3]{\frac{2ms_j}{\varepsilon^2}}\mathrm{Bi}'(z_j(x)) \end{pmatrix} \tag{15}$$

and

$$P_j \equiv \begin{pmatrix} 1 & 1 \\ i\kappa_j/\varepsilon & -i\kappa_j/\varepsilon \end{pmatrix}. \tag{16}$$

Then equation (14) can be rewritten as

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = P_j M_j(x_j)\begin{pmatrix} C_j^{(1)} \\ C_j^{(2)} \end{pmatrix}. \tag{17}$$

In the same way, we have at point $x_{j+1/2}$

$$M_j(x_{j+1/2} = x_j + \Delta x/2)\begin{pmatrix} C_j^{(1)} \\ C_j^{(2)} \end{pmatrix} = M_{j+1}(x_{j+1/2} = x_j + \Delta x/2)\begin{pmatrix} C_{j+1}^{(1)} \\ C_{j+1}^{(2)} \end{pmatrix} \tag{18}$$

and also at point x_{j+1}

$$M_{j+1}(x_{j+1})\begin{pmatrix} C_{j+1}^{(1)} \\ C_{j+1}^{(2)} \end{pmatrix} = P_{j+1}\begin{pmatrix} a_2 \\ b_2 \end{pmatrix}. \tag{19}$$

Combine all the equations above (17), (18) and (19) we have

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = P_j^{-1} M_j(x_j) M_j^{-1}(x_{j+1/2}) M_{j+1}(x_{j+1/2}) M_{j+1}^{-1}(x_{j+1}) P_{j+1}\begin{pmatrix} a_2 \\ b_2 \end{pmatrix}. \tag{20}$$

Notice the difference between $M_j(x_j)$ and $M_j^{-1}(x_{j+1/2})$, also the difference between $M_{j+1}(x_{j+1/2})$ and $M_{j+1}^{-1}(x_{j+1})$, thus these matrices can't be cancelled.

Finally, our M is

$$M = P_j^{-1} M_j(x_j) M_j^{-1}(x_{j+1/2}) M_{j+1}(x_{j+1/2}) M_{j+1}^{-1}(x_{j+1}) P_{j+1} \tag{21}$$

3 Conclusion

To calculate the transmission and reflection coefficients at $x_{j+1/2}$. First, we calculate M using (21) in which M_j and P_j are defined by (15) and (16). Then we calculate S using (5) to get r_1, $t1$, r_2 and t_2. Finally, apply (8) or (9) to get the result.