1 General Case

1. **Wavefunction solution from Schrodinger's equation**

Before proceeding to derive the prescribed problem set, we can first try to examine a more general case of the system. This may give us more insights in constructing the transfer matrix. We start by modifying the problem set a bit by instead considering the following potential configuration.

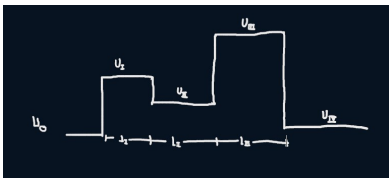

Figure 1: Arbitrary potential configuration

Calculation of the wavefunction is basically finding the solution of a boundary-value problem via Schrodinger's equation along a given interval. The boundary conditions are given by the behavior of two intersecting wavefunctions at a given boundary. The intersection must be continuous (wavefunctions must be equal at the boundary) and smooth (wavefunction derivatives must be equal at the boundary). It should be noted in the special case of a constant potential that the wavefunction can be expressed by an expression parametrized by the potential value and the particles energy. Hence, similar or different parameter values must correspond to similar or different wavefunctions.

The goal of this exercise is to express these conditions ultimately in a matrix form. This is such that a composite matrix can be calculated transforming an incoming wavefunction along any arbitrary sequence of potential steps. The matrix itself possesses properties of the wavefunction at the specified position in space such as transmission and reflection probability amplitude.

2. **Constant potential solution to Schrodinger's equation**

We proceed to derive a general solution to the time-independent Schrodinger equation (TISE) in the region n with constant potential V_n. We denote n as a roman numeral symbol. TISE reads

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_n(x)}{\mathrm{d}x} + V_n\psi_n(x) = E\psi_n(x) \tag{1}$$

This is simply a constant-coefficient second order ordinary differential equation which is easily recognizable in the form

$$\frac{\mathrm{d}^2\psi_n(x)}{\mathrm{d}x^2} = \frac{2m\left(V_n - E\right)}{\hbar^2}\psi_n(x) \tag{2}$$

which has a solution of form

$$\psi_n(x) = \tau_n \exp\left(ik_n x\right) + \gamma_n \exp\left(-ik_n x\right) \tag{3}$$

where τ_n and γ_n are arbitrary constants of integration and $k_n := \sqrt{(2m(E - V_n))/(\hbar^2)}$. Observe that the wavefunction in a given area n is parametrized by the constants τ_n and γ_n, and potential-dependent k_n. The key to note here is that two neighboring areas n and $n+1$ must have related constants τ_n, τ_{n+1}, γ_n, and γ_{n+1} due to continuity and smoothness conditions. Knowing the relationship between these neighboring constants at a given boundary, we can derive a function that converts a wavefunction from one constant potential to a neighboring constant potential. We proceed to derive this relationship in the next section.

3. **The Hopping Matrix**

From the solution of TISE expressed as in the Eq. (3), continuity requires $\psi_n(x) = \psi_{n+1}(x)$, while smoothness requires $\mathrm{d}\psi_n/\mathrm{d}x = \mathrm{d}\psi_{n+1}/\mathrm{d}x$ That is, in the boundary $x = m$ where m is denoted as a subscript $x_m = m$

$$\tau_n \exp(ik_n x_m) + \gamma_n \exp(-ik_n x_m) = \tau_{n+1} \exp(ik_{n+1} x_m) + \gamma_{n+1} \exp(-ik_{n+1} x_m) \tag{4}$$

$$ik_n \tau_n \exp(ik_n x_m) - ik_n \gamma_n \exp(-ik_n x_m) = ik_{n+1} \tau_{n+1} \exp(ik_{n+1} x_m) - ik_{n+1} \gamma_{n+1} \exp(-ik_{n+1} x_m) \tag{5}$$

These expressions can be compactified when converting them into a matrix form. Defining a vector $\vec{\psi}_n(x)$ as

$$\vec{\psi}_n(x) = \begin{bmatrix} \tau_n \exp(ik_n x) \\ \gamma_n \exp(-ik_n x) \end{bmatrix} \tag{6}$$

The conditions Eqs. (4) and (5) can be converted into a 2-dimensional linear system expressed compactly as

$$\begin{bmatrix} 1 & 1 \\ ik_n & -ik_n \end{bmatrix} \vec{\psi}_n(x_m) = \begin{bmatrix} 1 & 1 \\ ik_{n+1} & -ik_{n+1} \end{bmatrix} \vec{\psi}_{n+1}(x_m) \tag{7}$$

Hence, we can define a matrix $M(U_n, U_{n+1})$ such that

$$\vec{\psi_n}(x_m) = M(U_n, U_{n+1}) \vec{\psi_{n+1}} \tag{8}$$

We can find M by simply inverting the matrix

$$\vec{\psi_n}(x_m) = \begin{bmatrix} 1 + \frac{k_n}{k_{n+1}} & 1 - \frac{k_n}{k_{n+1}} \\ 1 - \frac{k_n}{k_{n+1}} & 1 + \frac{k_n}{k_{n+1}} \end{bmatrix} \vec{\psi}_{n+1} \tag{9}$$

where we can define

$$M_h(U_{n+1}, U_n) := \frac{1}{2} \begin{bmatrix} 1 + \frac{k_n}{k_{n+1}} & 1 - \frac{k_n}{k_{n+1}} \\ 1 - \frac{k_n}{k_{n+1}} & 1 + \frac{k_n}{k_{n+1}} \end{bmatrix} \tag{10}$$

4. **The Running Matrix**

We have derived a matrix that can transform a wavefunction from a potential to another given only the potential difference. However, note that this can only be used at the boundaries between each potential. We still need to traverse the constant potential itself. Similarly, we can also derive a matrix as follows. Doing this allows us to remain in a region n and use the same wavefunction. Consider the two non-boundary points $x_{m1} = m_1$ and $x_{m2} = m_2$ in the region n. Then,

$$\vec{\psi}_n(x_{m1}) = \begin{bmatrix} \tau_n \exp(ik_n x_{m1}) \\ \gamma_n \exp(-ik_n x_{m1}) \end{bmatrix} \qquad \vec{\psi}_n(x_{m2}) = \begin{bmatrix} \tau_n \exp(ik_n x_{m2}) \\ \gamma_n \exp(-ik_n x_{m2}) \end{bmatrix} \tag{11}$$

To transform $\vec{\psi}_n(x_{m1})$ into $\vec{\psi}_n(x_{m2})$, a trivial transformation can be used.

$$\begin{bmatrix} \tau_n \exp(ik_n x_{m1}) \\ \gamma_n \exp(-ik_n x_{m1}) \end{bmatrix} = \begin{bmatrix} \exp(ik_n(x_{m2} - x_{m1})) & 0 \\ 0 & \exp(-ik_n(x_{m2} - x_{m1})) \end{bmatrix} \begin{bmatrix} \tau_n \exp(ik_n x_{m2}) \\ \gamma_n \exp(-ik_n x_{m2}) \end{bmatrix} \tag{12}$$

But $x_{m2} - x_{m1}$ is simply the length of the region n we denote as L_n. Hence,

$$\vec{\psi}_n(x_{m2}) = \begin{bmatrix} \exp(ik_n L_n) & 0 \\ 0 & \exp(-ik_n L_n) \end{bmatrix} \vec{\psi}_n(x_{m1}) \tag{13}$$

where we can define

$$M_r(L_n, U_n) := \begin{bmatrix} \exp(ik_n L_n) & 0 \\ 0 & \exp(-ik_n L_n) \end{bmatrix} \tag{14}$$

This is the running matrix we denote as $M_r(L_n, U_n)$ which is dependent on the length L_n of the region of constant potential U_n.

5. **The Transfer Matrix**

To transfer from one general point to another, one simply needs to "run" through the length L_n of a constant potential U_n using M_r and "hop" from potential U_n across U_{n+1} using M_h. That is, to find the composite transfer matrix, we perform these runs and hops by repeatedly multiplying the vector $\vec{\psi}_n$ by the appropriate matrix. Of course, one needs to keep in mind that the potential U_n is conveniently stored in k_n. We can compose the first events: entering the first potential entrance and traversing the first potential.

$$\vec{\psi_2}(x) = M_r(L_1, U_1)M_h(U_0, U_1)\vec{\psi_0}(x) \tag{15}$$

This converts the wavefunction of incoming wave (region 0) into the wavefunction in the (region 2). We can compose the matrices as

$$M_r(L_1, U_1)M_h(U_0, U_1) = \prod_{n_0=0}^{n_f=2} M_r(L_{n+1}, U_{n+1})M_h(U_n, U_{n+1}) \tag{16}$$

Hence, if we define a general transfer matrix as

$$M_t(n_0, n_f) := \prod_{n=n_0}^{n_f} M_r(L_{n+1}, U_{n+1})M_h(U_n, U_{n+1}) \tag{17}$$

we can first calculate the transfer matrix of a given potential configuration and parametrize it with respect to physical parameters (E, m). Again, this matrix allows us to enter one potential and exit through another. That is

$$\vec{\psi}_{n_0}(x) = M_t(n_0, n_f)\vec{\psi}_{n_f}(x) \tag{18}$$

M_t encodes properties of the potential (its configuration shape as dictated by steepness and width of each individual well) and properties of the particle (mass and energy).

2 Answers to Problem Set 5

1. **Wavefunction solution from Schrodinger's equation**

   Thanks to our results, we can now prove the following relations as is tasked in this problem set. Proving these is tantamount to reducing our general results to the specified potential configuration below.

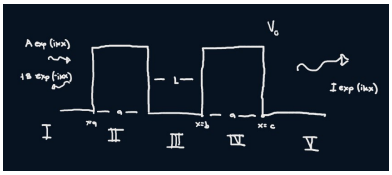

Figure 2: Double barrier potential with equal heights

Show that :

- in region II, for $E < V_0$, $\psi = C \exp(-\beta x) + D \exp(\beta x)$ where $\beta = \sqrt{2m(V_0 - E)/\hbar^2}$
- in region III, for $E < V_0$, $\psi = F \exp(ikx) + G \exp(-ikx)$ where $k = \sqrt{2mE/\hbar^2}$

Recall that from Eq. (3), the general solution for TISE at region n is

$$\psi_n(x) = \tau_n \exp(ik_n x) + \gamma_n \exp(-ik_n x)$$

where $k_n := \sqrt{(2m(E - V_n))/\hbar^2}$. At region II, we see that $\tau_n = D$, $\gamma_n = C$, and $ik_n = \beta$. At region III, we see that $\tau_n = F$, $\gamma_n = G$, and $k_n = k$ (since the potential here is zero). This proves the proposed solutions to TISE at regions II and III.

2. **Region 0 - Region I Boundary Condition**

Show that the boundary conditions at $x = 0$ is

$$\begin{aligned} A + B &= C + D \\ ik(A - B) &= \beta(D - C) \end{aligned}$$

[a] or

$$\begin{bmatrix} 1 & 1 \\ ik & -ik \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \beta & -\beta \end{bmatrix} \begin{bmatrix} D \\ C \end{bmatrix}$$

[a] C was denoted as E in the problem set questionnaire.

Observe the k_0 is not equal to k_I since the potential at region 0 is not equal to the potential at region I. We can see this more clearly when we recall Eqs. (4) and (5). Since $k_n \neq k_{n+1}$, it might seem that we need to factor in the exponentials. However, upon closer inspection, both exponentials are evaluated at $x = 0$ and thus must vanish to unity. Hence, we are left with an equation of coefficients. We can see that letting $\tau_n = A$, $\gamma_n = B$, $\tau_{n+1} = D$, $\gamma_{n+1} = C$, $ik_n = ik$, and $ik_{n+1} = \beta$, the general case reduces to this specific boundary condtions. Invoking our result from Eq. (7) and these substitutions, we can clearly see that the system of equations and its matrix representation hold. Note that these coefficients came directly from the definition at Eq. (6)

3. **Region I - Region II Boundary Condition**

Show that the boundary conditions at $x = a$ is

$$D\exp(\beta a) + C\exp(-\beta a) = F\exp(ika) + G\exp(-ika)$$
$$\beta(D\exp(\beta a) - C\exp(-\beta a)) = ik(F\exp(ika) + G\exp(-ika))$$

or

$$\begin{bmatrix} \exp(\beta a) & \exp(-\beta a) \\ \beta\exp(\beta a) & -\beta\exp(-\beta a) \end{bmatrix} \begin{bmatrix} D \\ C \end{bmatrix} = \begin{bmatrix} \exp(ika) & \exp(-ika) \\ ik\exp(ika) & -ik\exp(-ika) \end{bmatrix} \begin{bmatrix} F \\ G \end{bmatrix}$$

Showing that the boundary conditions hold is tantamount to finding the appropriate conversion of coefficients and constants from Eqs. (4) and (5). We see that if we define an ordered 6-tuple $\{\tau, \gamma, \tau_{n+1}, \gamma_{n+1}, k_n, k_{n+1}\}$, the point (D, C, F, G, β, k) gives us the boundary conditions at $x = a$. There is some slight difference with the general form. Observe that the exponential parts have been absorbed into the matrices themselves leaving the vector with only the coefficients as elements. In this form, we need to redo matrix inversion. Inverting the matrix and multiplying both sides by the inverse,

$$\begin{bmatrix} D \\ C \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\exp(ika - a\beta) & \frac{1}{2\beta}\exp(-ika - a\beta) \\ \frac{1}{2}ik\exp(ika + a\beta) & \frac{1}{2\beta}\exp ik(-ika + a\beta) \end{bmatrix} \begin{bmatrix} F \\ G \end{bmatrix} \tag{19}$$

4. **Hopping Matrix at x=0**

Find the constant potential transition matrix M_0 where

$$M_0 \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}$$

Recall that at x = 0 , $k_n = k$ and $k_{n+1} = \beta$. Plugging in, we see that the hopping matrix at $x = 0$ is

$$M_s(U_n, U_{n+1}) = \frac{1}{2}\begin{bmatrix} 1 + \frac{k}{\beta} & 1 - \frac{k}{\beta} \\ 1 - \frac{k}{\beta} & 1 + \frac{k}{\beta} \end{bmatrix} \tag{20}$$

5. **Hopping Matrix at x=a**

Find the potential step transition matrix M_s where

$$M_s \begin{bmatrix} D \\ C \end{bmatrix} = \begin{bmatrix} F \\ G \end{bmatrix}$$

Similarly, at x=a, we take our recently inverted matrix. That is,

$$\begin{bmatrix} \frac{1}{2}\exp(ika - a\beta) & \frac{1}{2\beta}\exp(-ika - a\beta) \\ \frac{1}{2}ik\exp(ika + a\beta) & \frac{1}{2\beta}\exp ik(-ika + a\beta) \end{bmatrix} \tag{21}$$

6. **Tranfer Matrix from Region I to Region V**

Find the potential step transition matrix M_s where

$$M_s \begin{bmatrix} D \\ C \end{bmatrix} = \begin{bmatrix} F \\ G \end{bmatrix}$$

Observed that I have restructured the construction of the transfer matrix. The problem set instructs us to propagate the defined vector $\vec{v} = (\tau_n, \gamma_n)$ with only the coefficients as elements. Hence, the hopping and running matrices would contain exponential terms as we have observed at Eq. (**??**). It would be more intuitive to compose the matrices as was derived in the first chapter with the general case as we can

clearly see the hops and runs of the wavefunction itself. The plan is to compose the transfer matrix T this way and to extract the probabilities in the end. To do so, we simply use our result from Eq. (22).

$$M_t(n_0, n_f) := \prod_{n=n_0}^{n_f} M_r(L_{n+1}, k_{n+1}) M_h(k_n, k_{n+1}) \tag{22}$$

Explicitly, we hop at $x = 0$, run towards $x = a$, hop at $x = a$, run towards $x = b$, hop at $x = b$, run towards $x = c$, and hop at $x = c$. To do so, we need to compile the wavenumber k and the length L for each region. At region I, $k_I = k$.[1]. At region II, $k_{II} = \beta$, $L_{II} = a$. At region III, $k_{III} = k$, $L_{III} = L$. At region IV, $k_{IV} = \beta$, $L_{IV} = a$. Finally at region V, $k_V = k$. The transfer matrix from $x = 0$ to $x = c$ is then,

$$T(0, c) = M_h(k, \beta) M_r(a, \beta) M_h(\beta, k) M_r(L, k) M_h(k, \beta) M_r(a, \beta) M_h(\beta, k) \tag{23}$$

Note that the transfer matrix is a function of the potential configuration and the particle's parameters. We can reparametrize the wavefunction vector with respect to the initial amplitude. Due to linearity of the TISE PDE,

$$\vec{\psi}(0) = A \begin{bmatrix} 1 \\ r \end{bmatrix} \qquad \vec{\psi}(c) = A \begin{bmatrix} t \\ 0 \end{bmatrix} \tag{24}$$

where A is the amplitude of rightward incoming wave, Ar is the amplitude of leftward reflection wave[2], At is the amplitude of rightward transmitted wave[3], and 0 is the amplitude of the non-existent leftward incoming wave. Using these parametrization for convenience, we now have the relation

$$A \begin{bmatrix} t \\ 0 \end{bmatrix} = T(0, c) A \begin{bmatrix} 1 \\ r \end{bmatrix} \iff \begin{bmatrix} t \\ 0 \end{bmatrix} = T(0, c) \begin{bmatrix} 1 \\ r \end{bmatrix} \tag{25}$$

from where we can easily extract the values of r and t. We borrow the results Y. D. Chong and find that

$$R = \frac{T_{21}}{T_{22}} \tag{26}$$

$$T = \frac{\det(\mathrm{T})}{T_{22}} \tag{27}$$

The transfer matrix T at Eq. (23) is a successive matrix multiplication and quite messy to do. After all, transfer matrices as usually used to calculate things numerically. However, several observations can be made from Eq. (23) listed below:

I $M_h(k, \beta) = (M_h(\beta, k))^{-1}$
II $M_h(k, \beta) \cdot M_r(a, \beta)) = M_r(a, \beta) \cdot M_h(\beta, k)$

One can easily see these properties to hold if one visualizes the intuitive notion of transfer matrices as propagating the wavefunction segment by segment. Using these properties, we can recast Eq. (23) as

$$\begin{aligned} T(0, c) &= M_h(k, \beta) M_h(\beta, k) M_r(a, \beta) M_r(L, k) M_r(a, \beta) M_h(k, \beta) M_h(\beta, k) && (28) \\ &= M_r(a, \beta) M_r(L, k) M_r(a, \beta) && (29) \end{aligned}$$

where a quick matrix multiplication gives us

$$T(0, c) = \begin{bmatrix} \exp\ i(kL + 2a\beta) & 0 \\ 0 & \exp\ -i(kL + 2a\beta) \end{bmatrix} \tag{30}$$

We can observe that the final transfer matrix is a diagonal matrix. Moreover, it has complex conjugate diagonal elements. This gives us a unit determinant. Using Eqs. (26) and (27), we have that this configuration possesses a transparent $T = 1$ transmission probability. It is also interesting to note that such resonant tunnelling transparency is energy-independent. This was a direct consequence of property I and the $k - \beta \to \beta - k$ symmetry.

[1] I apologize for the abuse of notation. I have defined similar variables as the given constants and have only noticed it later.
[2] In the problem set, this was given as B
[3] In the problem set, this was given as I