33 Methods for one-dimensional problems

Slides: Lecture 33a Introduction to methods for one-dimensional problems

Text reference: Quantum Mechanics for Scientists and Engineers

Chapter 11 introduction
Methods for one-dimensional problems
33 Methods for one-dimensional problems

Slides: Lecture 33b Tunneling currents

Text reference: Quantum Mechanics for Scientists and Engineers
Section 11.1
Tunneling rates

Consider a simple rectangular barrier with incident electron energy $E$ below the (peak) barrier height $V_o$, i.e., $E < V_o$.

We also presume no electrons incident from the right so there are only transmitted electrons there.
Tunneling rates

We could have a more complicated barrier still with $E < V_0$ but possibly with a different potential on the right and different wavevector $k_R$.

incident electrons

reflected electrons

transmitted electrons

$$\psi_L(z) = Ae^{ikz} + Be^{-ikz}$$

$$\psi_R(z) = Fe^{ik_Rz}$$
Tunneling rates

Suppose we have found the relations between the amplitudes of the incident, $A$, reflected, $B$, and transmitted, $F$, waves

incident electrons $\rightarrow$ reflected electrons $\leftarrow$ transmitted electrons

\[
\begin{align*}
\psi_L(z) &= Ae^{ikz} + Be^{-ikz} \\
\psi_B(z) &= Ce^{-\kappa z} + De^{\kappa z} \\
\psi_R(z) &= Fe^{ikz}
\end{align*}
\]

$-L_z/2$ $\rightarrow$ $L_z/2$
Suppose we have found the relations between the amplitudes of the incident, $A$, reflected, $B$, and transmitted, $F$, waves in either case. How do we relate these to actual electron currents?
Evaluation of tunneling current

The particle current density in quantum mechanics is

$$ j_p = \frac{i\hbar}{2m} (\Psi \nabla \Psi^* - \Psi^* \nabla \Psi) $$

where $\Psi = \Psi(r, t)$ is the time-dependent wavefunction.

If we consider particles of well-defined energy $E$,
the wavefunction is of the form $\Psi(r, t) = \psi(r) \exp(-iEt / \hbar)$

In the products $\Psi \nabla \Psi^*$ and $\Psi^* \nabla \Psi$,
the term $\exp(-iEt / \hbar)$ is multiplied by its complex conjugate to give 1, so we then have

$$ j_p = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) $$
Evaluation of tunneling current

If we consider only a one-dimensional problem e.g., for a potential varying only in the $z$ direction we only need to calculate the current in the $z$ direction which we can call $j_p$

so we simplify $j_p = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi)$

to just

$$j_p = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi)$$

where $\psi = \psi(z)$ is now just a spatial wavefunction varying in $z$
Evaluation of tunneling current

For a simple barrier with the same potential on the left and the right which we take to be zero for simplicity for a particle of mass $m$ and energy $E$, we have, as usual

$$E = \frac{\hbar^2 k^2}{2m}$$

incident electrons
\[ \psi_L(z) = Ae^{ikz} + Be^{-ikz} \]
reflected electrons
\[ \psi_B(z) = Ce^{-\kappa z} + De^{\kappa z} \]
transmitted electrons
\[ \psi_R(z) = Fe^{ikz} \]
Evaluation of tunneling current

With the wave on the right in the form \( \psi_R(z) = F e^{ikz} \)

from \( j_p = \frac{i\hbar}{2m} \left( \psi \nabla \psi^* - \psi^* \nabla \psi \right) \)

noting that \( \psi \nabla \psi^* = |F|^2 \exp(ikz) \frac{d}{dz} \exp(-ikz) \)

\[ = -ik |F|^2 \]

and similarly \( \psi^* \nabla \psi = ik |F|^2 \)

we have \( j_p = |F|^2 \frac{\hbar k}{m} \)
Evaluation of tunneling current

On the left, with $\psi(z) = A \exp(ikz) + B \exp(-ikz)$ from $j_p = (i\hbar / 2m) \left( \psi \nabla \psi^* - \psi^* \nabla \psi \right)$ we have

$$j_p = \frac{i\hbar}{2m} \left\{ \left[ A \exp(ikz) + B \exp(-ikz) \right] \left[ -ikA^* \exp(-ikz) + ikB^* \exp(ikz) \right] \right\} \right.$$

$$= \frac{\hbar k}{m} \left( |A|^2 - |B|^2 \right)$$

Note that all the spatially oscillating terms cancel

The net current is not varying spatially on the left
Evaluation of tunneling current

Since we have deduced

\[ j_p = \left( \frac{\hbar k}{m} \right) \left( |A|^2 - |B|^2 \right) \]

we can therefore consider \( \hbar k |A|^2 / m \) as the forward current on the left and \( \hbar k |B|^2 / m \) as the reflected or backward current adding the two to get the net current
Relation to group velocity

For $E = \frac{\hbar^2 k^2}{2m} \equiv \hbar \omega$ where $\omega$ is the frequency associated with $E$, gives group velocity $v_g = \frac{d \omega}{dk} = \frac{\hbar k}{m}$

So the currents can be written:

\begin{align*}
\text{forward} & \quad \hbar k |A|^2 / m \equiv |A|^2 v_g \\
\text{backward} & \quad \hbar k |B|^2 / m \equiv |B|^2 v_g \\
\text{transmitted} & \quad \hbar k |F|^2 / m \equiv |F|^2 v_g
\end{align*}

though group velocity is not required for our argument
Evaluation of tunneling current

With these currents

- forward: $\frac{\hbar k |A|^2}{m}$
- backward: $\frac{\hbar k |B|^2}{m}$

the fraction transmitted by the barrier can be written as

$$\eta = \frac{\text{current not reflected}}{\text{incident forward current}} = \frac{|A|^2 - |B|^2}{|A|^2}$$

incident electrons

$\psi_L(z) = Ae^{ikz} + Be^{-ikz}$

reflected electrons

$\psi_B(z) = Ce^{-\kappa z} + De^{\kappa z}$

transmitted electrons

$\psi_R(z) = Fe^{ikz}$

$V_o$

$-L_z/2 \quad L_z/2$
Evaluation of tunneling current

It might seem more obvious to write, with currents

forward \( \hbar k |A|^2 / m \)

transmitted \( \hbar k |F|^2 / m \)

that the fraction transmitted is

\[
\eta = \frac{\text{current transmitted}}{\text{incident forward current}} = \frac{|F|^2}{|A|^2}
\]

\[
\psi_L(z) = Ae^{ikz} + Be^{-ikz}
\]

\[
\psi_B(z) = Ce^{-\kappa z} + De^{\kappa z}
\]

\[
\psi_R(z) = Fe^{ikz}
\]
Evaluation of tunneling current

For a barrier with the same potential and material on both sides, these two expressions

give the same answers:

\[
\eta = \frac{|A|^2 - |B|^2}{|A|^2} \quad \text{and} \quad \eta = \frac{|F|^2}{|A|^2}
\]
Tunneling rates

But with different potential or material on the right, the group velocity may be different on the right or might not be defined in some complicated case. While we might handle that, avoids these issues and is often otherwise just as easy to calculate.

\[ \eta = \frac{\left( |A|^2 - |B|^2 \right)}{|A|^2} \]

\[ \psi_L(z) = Ae^{ikz} + Be^{-ikz} \]

\[ \psi_R(z) = F e^{ik_Rz} \]
Evaluation of tunneling current

For example, in field-emission tunneling, the barrier may continue its slope, giving no constant group velocity on the right.

Here, however, still works

\[ \eta = \frac{|A|^2 - |B|^2}{|A|^2} \]

\[ \psi_L(z) = A e^{ikz} + B e^{-ikz} \]
33 Methods for one-dimensional problems

Slides: Lecture 33c Transfer matrix method

Text reference: Quantum Mechanics for Scientists and Engineers

Section 11.2 up to “Calculation of eigenenergies ...”
Methods for one-dimensional problems

Transfer matrix method

Quantum mechanics for scientists and engineers

David Miller
Transfer matrix method

We presume that the potential is a series of steps.
This could be an actual step-like potential
or we could be approximating some continuously varying potential.
Transfer matrix method

We therefore reduce the problem to that of waves within a simple constant potential which are either sinusoidal or exponential together with appropriate boundary conditions to link the solutions in adjacent layers.

Step-wise approximation to $V(z)$

Actual $V(z)$
Transfer matrix method

Consider an electron wave incident on the structure from one side, with a particular energy, $E$.

There will be reflected waves and transmitted waves.
Transfer matrix method

For each layer in the structure, we derive a matrix that relates the forward and backward amplitudes $A_m$ and $B_m$, just to the right of the $(m-1)$th interface, to $A_{m+1}$ and $B_{m+1}$, just to the right of the $m$th interface.

![Diagram of wave interaction through layers](image-url)
Transfer matrix method

By multiplying those matrices together for all of the layers we will construct a single "transfer matrix" for the whole structure enabling us to analyze the entire multilayer structure.

incident wave

reflected wave

transmitted wave

layer 1 2 3 4 ... N  N+1  N+2

interface 1 2 3 4 N  N-1  N+1
Transfer matrix method

In this formalism, each layer $m$ will have

- a potential energy $V_m$
- a thickness $d_m$
- and possibly a mass or effective mass $m_{fm}$

incident wave

reflected wave

transmitted wave

\[ V_1 d_2 V_2 d_3 V_3 d_4 V_4 \ldots V_N d_N V_{N+1} V_{N+2} \]
Transfer matrix method

For interfaces 2 and higher, the position of the $m$th interface relative to interface 1, e.g., $z_2 = d_2$, $z_3 = d_2 + d_3$, etc., is

$$z_m = \sum_{q=2}^{m} d_q$$
Transfer matrix method

In any given layer, if the particle energy $E > V_m$ we know we will have in general both

a "forward" propagating wave $A = A_o \exp[i k_m (z - z_{m-1})]$ and

a "backward" propagating wave $B = B_o \exp[-i k_m (z - z_{m-1})]$ where $A$ and $B$ are complex numbers for the forward and backward wave amplitudes

In this case

$$k_m = \sqrt{\frac{2m_{fm}}{\hbar^2}} (E - V_m)$$

where $m_{fm}$ is the mass of the particle in that layer
Transfer matrix method

Similarly, if the particle energy $E < V_m$ we know we will have in general both a "forward" decaying "wave" 

$$A = A_o \exp\left[-\kappa_m (z - z_{m-1})\right]$$

and

a "backward" decaying "wave" 

$$B = B_o \exp\left[\kappa_m (z - z_{m-1})\right]$$

where $A$ and $B$ are complex numbers for the forward and backward "wave" amplitudes.

In this case

$$\kappa_m = \sqrt{\frac{2m_{fm}}{h^2}(V_m - E)}$$

where $m_{fm}$ is the mass of the particle in that layer.
Transfer matrix method

Note that for $E < V_o$ if we use the form $k_m = \sqrt{\frac{2m_{fm}}{\hbar^2}}(E - V_m)$
we obtain an imaginary $k_m$
As long as we choose the positive square root (either real or imaginary) in both cases
we can work with only this form
For example, a forward propagating “wave” can then be written in the form $\exp\left[ ik_m (z - z_{m-1}) \right]$
for both cases $E < V_o$ and $E > V_o$
and similarly for the backward propagating “wave”
Transfer matrix method

Now in any layer we have a wave that we can write as

$$\psi(z) = A_m \exp[i k_m (z - z_{m-1})] + B_m \exp[-i k_m (z - z_{m-1})]$$

where $k_m$ can be either real or imaginary and is given by

$$k_m = \sqrt{\frac{2m_{fm}}{\hbar^2}(E - V_m)}$$

This can greatly simplify the algebra for this method.
Boundary conditions

Now let us look at the boundary conditions in going from just inside one layer to the right of the boundary to just inside the adjacent layer on the left of the boundary. For a reason that will become apparent later, we will work from right to left in setting these up.

\[
\begin{align*}
\text{layer} & \quad m & \quad \text{layer} & \quad m+1 \\
A_m & \to & A_L & \leftarrow A_{m+1} \\
B_m & \leftarrow & B_L & \to B_{m+1} \\
d_m & & & \\
& \text{interface} & m & \text{interface} & m+1
\end{align*}
\]
Boundary conditions

Using the notation of the figure for continuity of the wavefunction

\[ \psi = A_L + B_L = A_{m+1} + B_{m+1} \]

for the continuity of \( d\psi / dz \)

on either side of the boundary

\[ \frac{d\psi}{dz} = ik(A - B) \]

so at the right interface

\[ A_L - B_L = \Delta_m (A_{m+1} - B_{m+1}) \]

where

\[ \Delta_m = k_{m+1} / k_m \]
Boundary conditions

In a layered semiconductor structure we might use continuity of \( \frac{1}{m_f} \frac{d\psi}{dz} \) for the second boundary condition in which case we would obtain

\[
\Delta_m = \frac{k_{m+1} m_f m}{k_m m_f m+1}
\]

and we would use this \( \Delta_m \) in all subsequent algebra here.
Boundary conditions

Using \( A_L + B_L = A_{m+1} + B_{m+1} \) and

\[ A_L - B_L = \Delta_m \left( A_{m+1} - B_{m+1} \right) \]

gives

\[ A_L = A_{m+1} \left( \frac{1 + \Delta_m}{2} \right) + B_{m+1} \left( \frac{1 - \Delta_m}{2} \right) \]

and

\[ B_L = A_{m+1} \left( \frac{1 - \Delta_m}{2} \right) + B_{m+1} \left( \frac{1 + \Delta_m}{2} \right) \]
Boundary conditions

\[ A_L = A_{m+1} \left( \frac{1+\Delta_m}{2} \right) + B_{m+1} \left( \frac{1-\Delta_m}{2} \right) \]

and \[ B_L = A_{m+1} \left( \frac{1-\Delta_m}{2} \right) + B_{m+1} \left( \frac{1+\Delta_m}{2} \right) \]

can be written in matrix form as

\[
\begin{bmatrix}
A_L \\
B_L
\end{bmatrix} = D_m \begin{bmatrix}
A_{m+1} \\
B_{m+1}
\end{bmatrix} \quad D_m = \begin{bmatrix}
\frac{1+\Delta_m}{2} & \frac{1-\Delta_m}{2} \\
\frac{1-\Delta_m}{2} & \frac{1+\Delta_m}{2}
\end{bmatrix}
\]

layer \( m \)  \quad layer \( m+1 \)

\[ A_m \rightarrow A_L \quad A_{m+1} \]

\[ B_m \leftarrow B_L \quad B_{m+1} \]

interface \( m \)  \quad interface \( m+1 \)

\[ d_m \]
Now we treat the propagation that relates $A_m$ and $B_m$ to $A_L$ and $B_L$

For a minor formal reason, we calculate the matrices for going "backwards" through the structure.

For the propagation in layer $m$ with thickness $d_m$, we have

\[
A_m = A_L \exp(-i k_m d_m) \quad B_m = B_L \exp(i k_m d_m)
\]
Propagation matrix

These relations \( A_m = A_L \exp(-ik_m d_m) \)
\( B_m = B_L \exp(i k_m d_m) \)
can be written in matrix form as

\[
\begin{bmatrix}
A_m \\
B_m
\end{bmatrix} = P_m \begin{bmatrix}
A_L \\
B_L
\end{bmatrix}
\]

with

\[
P_m = \begin{bmatrix}
\exp(-ik_m d_m) & 0 \\
0 & \exp(i k_m d_m)
\end{bmatrix}
\]
The full transfer matrix, $T$, for the structure relates forward, $A_1$, and backward, $B_1$, “entrance” amplitudes i.e., just to the left of the first interface to forward, $A_{N+2}$, and backward, $B_{N+2}$, “exit” amplitudes i.e., just to the right of the last interface

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = T \begin{pmatrix} A_{N+2} \\ B_{N+2} \end{pmatrix} \quad \text{where} \quad T = D_1 P_2 D_2 P_3 D_3 \ldots P_{N+1} D_{N+1}$$

Note that this transfer matrix depends on the energy $E$ we chose for the calculation of the $k$’s in each layer
Full transfer matrix

\[
\begin{bmatrix}
A_1 \\
B_1
\end{bmatrix}
= 
T
\begin{bmatrix}
A_{N+2} \\
B_{N+2}
\end{bmatrix}
\]
and the product

\[
T = D_1 P_2 D_2 P_3 D_3 \cdots P_{N+1} D_{N+1}
\]

we move progressively from right to left

<table>
<thead>
<tr>
<th>propagation matrix</th>
<th>P_2</th>
<th>P_3</th>
<th>P_4</th>
<th>\ldots</th>
<th>P_N</th>
<th>P_{N+1}</th>
</tr>
</thead>
<tbody>
<tr>
<td>boundary condition</td>
<td>D_1</td>
<td>D_2</td>
<td>D_3</td>
<td>D_4</td>
<td>D_{N-1}</td>
<td>D_N</td>
</tr>
</tbody>
</table>

\[
\begin{bmatrix}
A_1 \\
B_1
\end{bmatrix}
= \begin{bmatrix}
T_1 & T_2 & T_3 & T_4 & \cdots & T_N \\
N & N+1 & N+2
\end{bmatrix}
\]

layer 1 \quad 2 \quad 3 \quad 4 \quad \ldots \quad N \quad N+1 \quad N+2

interface 1 \quad 2 \quad 3 \quad 4 \quad N-1 \quad N \quad N+1
Calculation of tunneling rates

Having calculated the transfer matrix \( T \equiv \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \)
for some structure and energy \( E \)
we now deduce the fraction of incident particles at that energy that are transmitted by the barrier.
We presume no wave incident from the right, so there is no backward wave amplitude on the right.
Hence, for incident forward and backward amplitudes \( A \) and \( B \) respectively,
and a transmitted amplitude \( F \)
\[
\begin{bmatrix} A \\ B \end{bmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{bmatrix} F \\ 0 \end{bmatrix}
\]
Calculation of tunneling rates

From

\[
\begin{bmatrix}
A \\
B
\end{bmatrix} =
\begin{bmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22}
\end{bmatrix}
\begin{bmatrix}
F \\
0
\end{bmatrix}
\]

we see that \( A = T_{11}F \) and \( B = T_{21}F \)

and hence the fraction of particles transmitted by this barrier is

\[
\eta = \frac{|A|^2 - |B|^2}{|A|^2} = 1 - \frac{|T_{21}|^2}{|T_{11}|^2}
\]

This approach is well suited for numerical calculations being straightforward to program.

It is a very useful practical technique for investigating one-dimensional potentials and their behavior.
Calculation of wavefunctions

Note that this method also enables us to calculate the wavefunction at any point in the structure.

We can readily calculate forward and backward amplitudes, $A_m$ and $B_m$, at the left of each layer.

Obviously, we have

$$
\begin{bmatrix}
A_{N+1} \\
B_{N+1}
\end{bmatrix} = P_{N+1}D_{N+1} \begin{bmatrix}
A_{N+2} \\
B_{N+2}
\end{bmatrix}
$$

and similarly, we have in general for any layer within the structure

$$
\begin{bmatrix}
A_m \\
B_m
\end{bmatrix} = P_m D_m \ldots P_N D_N P_{N+1} D_{N+1} \begin{bmatrix}
A_{N+2} \\
B_{N+2}
\end{bmatrix}
$$
Calculation of wavefunctions

Given that we know the forward and backward amplitudes at the left of layer $m$ from

$$\begin{bmatrix} A_m \\ B_m \end{bmatrix} = P_m D_m \ldots P_N D_N P_{N+1} D_{N+1} \begin{bmatrix} A_{N+2} \\ B_{N+2} \end{bmatrix}$$

then the wavefunction at some point $z$ in that layer is the sum of the forward and backward wavefunctions as in

$$\psi(z) = A_m \exp\left[i k_m (z - z_m)\right] + B_m \exp\left[-i k_m (z - z_m)\right]$$
Calculation of wavefunctions

Note that we could calculate these forward and backward amplitudes as intermediate results if we progressively evaluate the forward and backward amplitudes for each successive layer as in

$$
\begin{bmatrix}
A_m \\
B_m
\end{bmatrix} = P_m D_m \begin{bmatrix}
A_{m+1} \\
B_{m+1}
\end{bmatrix}
$$

rather than evaluating the transfer matrix $T$ itself.

By choosing no inward wave on the right we can still calculate the transmission probability from

$$
\eta = \left( |A_1|^2 - |B_1|^2 \right) / |A_1|^2
$$
Tunneling through a double barrier

This structure shows a resonance in the tunneling probability (or transmission) where the incident energy coincides with the energy of a resonance in the structure.

If the barriers were infinitely thick, there would be an eigenstate approximately at the energy where the first resonance occurs.
33 Methods for one-dimensional problems

Slides: Lecture 33d Transfer matrix and bound states

Text reference: Quantum Mechanics for Scientists and Engineers

Section 11.2 from “Calculation of eigenenergies ...”
Methods for one-dimensional problems

Transfer matrix and bound states

Quantum mechanics for scientists and engineers

David Miller
Eigenenergies of bound states

It is possible to use the transfer matrix itself to find eigenstates in cases of truly bound states.

For example, if the first layer (layer 1) and last layer (layer $N+2$) are infinitely thick, and have potentials $V_1$ and $V_{N+2}$, there may be values of $E < V_1, V_{N+2}$ for which there are bound eigenstates.
Eigenenergies of bound states

The wavefunctions would be exponentially decaying into the first and last layers. So the forward amplitude on the left \( A_1 = 0 \) i.e., no exponentially growing wave to the left of the structure and the backward amplitude on the right \( B_{N+2} = 0 \) i.e., no exponentially growing wave to the right of the structure.
Eigenenergies of bound states

So for a bound eigenstate, we have

\[
\begin{bmatrix}
0 \\
B_1
\end{bmatrix} = T \begin{bmatrix}
A_{N+2} \\
0
\end{bmatrix} = \begin{bmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22}
\end{bmatrix} \begin{bmatrix}
A_{N+2} \\
0
\end{bmatrix}
\]

This can only be the case if

\[ T_{11} = 0 \]

This condition can be used
to solve analytically for
eigenenergies in simple structures
or in a numerical search for
eigenenergies by varying \( E \)
33 Methods for one-dimensional problems

Slides: Lecture 33e Penetration factor for slowly varying barriers

Text reference: Quantum Mechanics for Scientists and Engineers

Section 11.3
Methods for one-dimensional problems

Penetration factor for slowly varying barriers

Quantum mechanics for scientists and engineers

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Penetration factor for slowly varying barriers

Consider a slowly varying potential approximated as a series of steps.

For simplicity, we choose the “entering” and “exiting” materials as having the same energy.

"entering" material
incident wave
reflected wave

"exiting" material
transmitted wave
Penetration factor for slowly varying barriers

We presume for an energy $E$ of interest

$E \ll V_m$ for each layer inside the structure, and that we have chosen the layers sufficiently thin in our calculation so that

at least for interfaces within the structure, $k_m \approx k_{m+1}$
Penetration factor for slowly varying barriers

Then, for interfaces within the structure

the boundary condition matrix

\[
D_m = \begin{bmatrix}
\frac{1+\Delta_m}{2} & \frac{1-\Delta_m}{2} \\
\frac{1-\Delta_m}{2} & \frac{1+\Delta_m}{2}
\end{bmatrix}
\]

with \( \Delta_m = \frac{k_{m+1}}{k_m} \approx 1 \) by assumption

can be approximated as the identity matrix

\[
D_m \approx \begin{bmatrix}
\sim 1 & \sim 0 \\
\sim 0 & \sim 1
\end{bmatrix}
\]
Penetration factor for slowly varying barriers

With internal boundary condition matrices therefore approximated by identity matrices we can omit them, so the transfer matrix becomes

$$T = D_1 P_2 P_3 \cdots P_N P_{N+1} D_{N+1}$$

We have left in the boundary condition matrices for the beginning and end of the structure where the potential may be quite discontinuous
Product of diagonal matrices

Note that the product of two diagonal matrices is simply a diagonal matrix whose elements are the products of the corresponding diagonal elements.

For example

\[
\begin{bmatrix}
a & 0 \\
0 & c
\end{bmatrix}
\begin{bmatrix}
b & 0 \\
0 & d
\end{bmatrix} =
\begin{bmatrix}
ab & 0 \\
0 & cd
\end{bmatrix}
\]
Penetration factor for slowly varying barriers

Since the propagation matrices are all diagonal and previously shown to be of the form

\[ P_m = \begin{bmatrix} \exp(-ik_m d_m) & 0 \\ 0 & \exp(i k_m d_m) \end{bmatrix} \]

then

\[ P_2 P_3 \cdots P_N P_{N+1} = \begin{bmatrix} 1/G & \sim 0 \\ \sim 0 & G \end{bmatrix} \]

where

\[ G = \prod_{q=2}^{N+1} \exp(i k_q d_q) = \prod_{q=2}^{N+1} \exp(-\kappa_q d_q) = \exp\left(-\sum_{q=2}^{N+1} \kappa_q d_q\right) \]
Now, if we have chosen the layers to be sufficiently thin we may take the summation to be approximately equal to an integral, i.e.,

\[ \sum_{q=2}^{N+1} \kappa_q d_q \approx \int_{0}^{z_{\text{tot}}} \kappa(z) \, dz \]

where \( z_{\text{tot}} \) \( (= z_{N+1}) \) is the total structure thickness which is taken to start on the left at \( z = 0 \)

Hence

\[ G = \exp \left( - \int_{0}^{z_{\text{tot}}} \kappa(z) \, dz \right) = \exp \left( - \int_{0}^{z_{\text{tot}}} \sqrt{\frac{2m_f}{\hbar^2}} (V(z) - E) \, dz \right) \]

where \( V(z) \) is the potential as a function of position \( z \)
Penetration factor for slowly varying barriers

With first and last boundary condition matrices

\[ D_1 = \begin{bmatrix} 1 + \Delta_1 & 1 - \Delta_1 \\ \frac{1}{2} & \frac{1}{2} \\ \frac{1 - \Delta_1}{2} & \frac{1 + \Delta_1}{2} \end{bmatrix} \quad \text{and} \quad D_{N+1} = \begin{bmatrix} 1 + \Delta_{N+1} & 1 - \Delta_{N+1} \\ \frac{1}{2} & \frac{1}{2} \\ \frac{1 - \Delta_{N+1}}{2} & \frac{1 + \Delta_{N+1}}{2} \end{bmatrix} \]

then

\[ T = D_1 P_2 P_3 \cdots P_N P_{N+1} D_{N+1} \]

\[ = \begin{bmatrix} 1 + \Delta_1 & 1 - \Delta_1 \\ \frac{1}{2} & \frac{1}{2} \\ \frac{1 - \Delta_1}{2} & \frac{1 + \Delta_1}{2} \end{bmatrix} \begin{bmatrix} 1/G & \sim 0 \\ \sim 0 & G \end{bmatrix} \begin{bmatrix} 1 + \Delta_{N+1} & 1 - \Delta_{N+1} \\ \frac{1}{2} & \frac{1}{2} \\ \frac{1 - \Delta_{N+1}}{2} & \frac{1 + \Delta_{N+1}}{2} \end{bmatrix} \]
Penetration factor for slowly varying barriers

So

\[
T = \begin{bmatrix}
\frac{1+\Delta_1}{2} & \frac{1-\Delta_1}{2} \\
\frac{1-\Delta_1}{2} & \frac{1+\Delta_1}{2}
\end{bmatrix}
\begin{bmatrix}
\frac{1}{G} & \sim 0 \\
\sim 0 & G
\end{bmatrix}
\begin{bmatrix}
\frac{1+\Delta_{N+1}}{2} & \frac{1-\Delta_{N+1}}{2} \\
\frac{1-\Delta_{N+1}}{2} & \frac{1+\Delta_{N+1}}{2}
\end{bmatrix}
\]

\[
T \approx \begin{bmatrix}
\frac{1+\Delta_1}{2} & \frac{1-\Delta_1}{2} \\
\frac{1-\Delta_1}{2} & \frac{1+\Delta_1}{2}
\end{bmatrix}
\begin{bmatrix}
\left(\frac{1+\Delta_{N+1}}{2}\right) & \frac{1}{G} \\
\left(\frac{1-\Delta_{N+1}}{2}\right) & G
\end{bmatrix}
\begin{bmatrix}
\left(\frac{1+\Delta_{N+1}}{2}\right) & \frac{1}{G} \\
\left(\frac{1-\Delta_{N+1}}{2}\right) & G
\end{bmatrix}
\]

\[
T_{11} \approx \left(\frac{1+\Delta_1}{2}\right)\left(\frac{1+\Delta_{N+1}}{2}\right)\frac{1}{G} + \left(\frac{1-\Delta_1}{2}\right)\left(\frac{1-\Delta_{N+1}}{2}\right)G
\]
Penetration factor for slowly varying barriers

Since the barrier is presumed thick \( G \approx \exp \left( -\int_0^{z_{tot}} \kappa(z) \, dz \right) \) is presumed small, so

\[
T_{11} \approx \left( \frac{1 + \Delta_1}{2} \right) \left( \frac{1 + \Delta_{N+1}}{2} \right) \frac{1}{G} + \left( \frac{1 - \Delta_1}{2} \right) \left( \frac{1 - \Delta_{N+1}}{2} \right) G \approx \frac{(1 + \Delta_1)(1 + \Delta_{N+1})}{4G}
\]

From

\[
\begin{bmatrix}
A \\
B
\end{bmatrix} = \begin{bmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22}
\end{bmatrix} \begin{bmatrix}
F \\
0
\end{bmatrix}, \quad A = T_{11}F \text{ so } \eta = \frac{|F|^2}{|A|^2} = 1 / |T_{11}|^2
\]

So

\[
\eta \approx \frac{16}{\left| (1 + \Delta_1)(1 + \Delta_{N+1}) \right|^2} \exp \left( -2 \int_0^{z_{tot}} \sqrt{\frac{2m_f}{\hbar^2}} (V(z) - E) \, dz \right)
\]
Penetration factor for slowly varying barriers

In this frequently used expression for tunneling probability or “penetration factor”

\[
\eta \approx \frac{16}{\left|1 + \Delta_1 \right| \left|1 + \Delta_{N+1} \right|} \exp \left( -2 \int_0^{z_{tot}} \sqrt{\frac{2m_f}{\hbar^2}} (V(z) - E) \, dz \right)
\]

the prefactor contains the input and output boundary conditions and

the exponential approximately expresses the “penetration” within the barrier