The electron pass through the single(multi) barrier (barriers).

Transfer Matrix Technique

Let's consider the electron transition through the tunneling barrier in the tunnel junction
(see potential profile Fig.1). Consider the both cases $E_1 < U_b$ and $E_1 > U_b$.

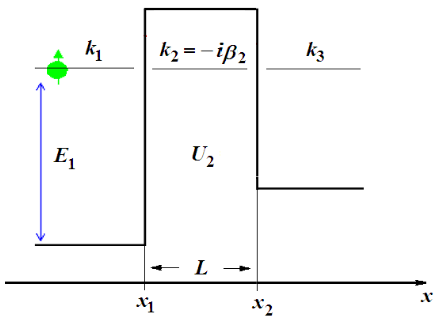


Fig.1 potential profile of the rectangular barrier.
The tunneling case is shown for $E_1 < U_b$, number of interfaces is 2.

General knowledge about tunneling and Transfer Matrix Technique

The motions states of the tunneling electrons (E) can be found from the solution of the homogeneous Shrödinger equation (1):

$$-\frac{\hbar^2}{2\,m}\frac{d^2}{dx^2}\Psi + (U(x) - E)\,\Psi = 0, \qquad (1)$$

or

$$\frac{d^2\,\Psi(x)}{dx^2} - \frac{2\,m}{\hbar^2}\,(U(x) - E)\,\Psi(x) = 0,$$

where $U(x)$ have to be constant in some region or piecewise continuous function. For E-energies, corresponding to the tunneling.

For example: $\frac{d^2\,\Psi_1(x)}{dx^2} - \frac{2\,m_1}{\hbar^2}\,(-E_1)\,\Psi_1(x) = 0$, (for left side of the junction); or

$$\frac{d^2\,\Psi_1(x)}{dx^2} + \frac{2\,m_1}{\hbar^2}\,(+E_1)\,\Psi_1(x) = 0$$

$\frac{d^2\,\Psi_2(x)}{dx^2} - \frac{2\,m_2}{\hbar^2}\,(U_b - E_1)\,\Psi_2(x) = 0$ (for the barrier); or

$$\frac{d^2\Psi_2(x)}{dx^2} + \frac{2\,m_2}{\hbar^2}(E_1 - U_b)\,\Psi_2(x) = 0$$

$$\frac{d^2\Psi_3(x)}{dx^2} - \frac{2\,m_3}{\hbar^2}(U_3 - E_1)\,\Psi_3(x) = 0$$ (for the right-side); or

$$\frac{d^2\Psi_3(x)}{dx^2} + \frac{2\,m_3}{\hbar^2}(E_1 - U_3)\,\Psi_3(x) = 0$$

$\frac{2\,m_r}{\hbar^2}=c_r$ - dimensional coefficient, or like this: $\frac{2\,m_r * m_0}{\hbar^2\,m_0}=c_0 M_{\text{eff}}$, where c_0= 0.2624 1/[(eV)*(Å^2)] and $M_{\text{eff}}=m_r/m_0$, m_0 is free electron mass.

The solution (1) in the regions 1 and 3 can be presented as follows:

$$\Psi_r(x) = A_r \exp(I\,k_r\,x) + B_r \exp(-I\,k_r\,x)\,, \qquad (2)$$

I is imaginary unit, r – is index of the region (For the single barrier model : r = 1, 2 and 3)

in common case r = 1, 2, 3, .., N

Applying the boundary conditions (BCs) :

$$\frac{1}{m_i}\,\partial_x \Psi_i(x_i) = \frac{1}{m_{i+1}}\,\partial_x \Psi_{i+1}(x_i)\,,\ \text{and also}$$

$$\Psi_i(x_i) = \Psi_{i+1}(x_i)\,,$$

where $i = 1, 2, .., n$, where n is the mount of interfaces, $n = N - 1$ and thus $N = n + 1$.

The coordinate of interfaces is determined as $x = x_i$

BCs give $2\,n$ number of equations,

the matrix form of this equations is :

Take $i = 1$ for the first interface ($x = x_1$), we have :

$$\begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}\begin{pmatrix} A_i \\ B_i \end{pmatrix} = \begin{pmatrix} a_5 & a_6 \\ a_7 & a_8 \end{pmatrix}\begin{pmatrix} A_{i+1} \\ B_{i+1} \end{pmatrix} \rightarrow \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} a_5 & a_6 \\ a_7 & a_8 \end{pmatrix}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

Take $i = 2$ for the second interface ($x = x_2$) and have :

$$\begin{pmatrix} a_9 & a_{10} \\ a_{11} & a_{12} \end{pmatrix}\begin{pmatrix} A_i \\ B_i \end{pmatrix} = \begin{pmatrix} a_{13} & a_{14} \\ a_{15} & a_{16} \end{pmatrix}\begin{pmatrix} A_{i+1} \\ B_{i+1} \end{pmatrix} \rightarrow \begin{pmatrix} a_9 & a_{10} \\ a_{11} & a_{12} \end{pmatrix}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} a_{13} & a_{14} \\ a_{15} & a_{16} \end{pmatrix}\begin{pmatrix} A_3 \\ B_3 \end{pmatrix}$$

where the coefficients a_1 .. a_8 contain x_1

(x_1 = 0 if you make the origin of x – axis in this point); a_9 .. a_{16} contain x_2

Or it can be represented in the following matrix form in general case

$$Q_j\begin{pmatrix} A_i \\ B_i \end{pmatrix} = Q_{j+1}\begin{pmatrix} A_{i+1} \\ B_{i+1} \end{pmatrix} \leftrightarrow \begin{pmatrix} a_p & a_{p+1} \\ a_{p+2} & a_{p+3} \end{pmatrix}\begin{pmatrix} A_i \\ B_i \end{pmatrix} = \begin{pmatrix} a_{p+4} & a_{p+5} \\ a_{p+6} & a_{p+7} \end{pmatrix}\begin{pmatrix} A_{i+1} \\ B_{i+1} \end{pmatrix}$$

for $n = 2$ and $N = 3$ it gives $j = 1$ and $j = 3$;

In common case the maximal j = $(2\,n - 1)$,

and it is odd numbers $j = 1, 3, 5, .. (2\,n - 1)$.

and total amount of the matrixes is the same as the number of equations,

which is $2\,n$ and we have the set $\{Q_1, Q_2, .., Q_{(2\,n)}\}$

p is index which numerate the matrix elements : when $i = 1$ then $p = 1$,
when $i = 3$ index p becomes $p = 9$ or in common case $p = 8\,i - 7$
As a result, the relation between amplitudes in region $r =$
1 and $r = 3$ is $\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \text{Inverse}[Q_1]\, Q_2\, \text{Inverse}[Q_3]\, Q_4 \begin{pmatrix} A_3 \\ B_3 \end{pmatrix}$;
In common case : it will be : $\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} =$
$\text{Inverse}[Q_1] \times Q_2 \times \,..\, \text{Inverse}[Q_x] \times Q_{x+1} \,..\times \text{Inverse}[Q_{2\,n-1}] \times Q_{2\,n} \begin{pmatrix} A_N \\ B_N \end{pmatrix}$
Remind that r, i, j, x are indexes
So, our interest is element $g_{11} = G_{[[1,1]]}$ of the matrix,
keeping in mind that set $\{a_1,\ a_2,\ a_3\ ..\ a_{(8\,n)}\}$ is found.
$G = \text{Inverse}[Q_1] \times Q_2 \times \,..\, \text{Inverse}[Q_x] \times Q_{x+1} \,..\times \text{Inverse}[Q_{2\,n-1}] \times Q_{2\,n}$
and
$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = G \begin{pmatrix} A_N \\ B_N \end{pmatrix},$$
$G[[1,\ 1]]$ element is the result for us, because it connects A_1 with A_N
$$\text{Transmission} = \frac{m_1}{m_N}\,\frac{k_N}{k_1} * \frac{|A_N|^2}{|A_1|^2}$$
TransmissionForSimpleBarrier = m1 / m3 * k3 / k1 * 1 / (G[[1, 1]] * Conjugate[G[[1, 1]]),
where m1 $= m_1$ and m3 $= m_3$ are effective electron mass,
k_1 is Fermi wave number for $r = 1$, k_3 is Fermi wave number for $r = 3$.

Program-Example of Transfer Matrix tech:
finding the Transmission as a function of energy E for rectangle barrier:

```
ClearAll;
a1 = k1[E1, m1] / m1 * Exp[I * k1[E1, m1] * x1];
a2 = -k1[E1, m1] / m1 * Exp[-I * k1[E1, m1] * x1];
a5 = k2[E1, Ub, m2] / m2 * Exp[I * k2[E1, Ub, m2] * x1];
a6 = -k2[E1, Ub, m2] / m2 * Exp[-I * k2[E1, Ub, m2] * x1];

a3 = Exp[I * k1[E1, m1] * x1];
a4 = Exp[-I * k1[E1, m1] * x1];
a7 = Exp[I * k2[E1, Ub, m2] * x1];
a8 = Exp[-I * k2[E1, Ub, m2] * x1];

a9 = k2[E1, Ub, m2] / m2 * Exp[I * k2[E1, Ub, m2] * x2];
a10 = -k2[E1, Ub, m2] / m2 * Exp[-I * k2[E1, Ub, m2] * x2];
a13 = k3[E1, V, m3] / m3 * Exp[I * k3[E1, V, m3] * x2];
a14 = -k3[E1, V, m3] / m3 * Exp[-I * k3[E1, V, m3] * x2];

a11 = Exp[I * k2[E1, Ub, m2] * x2];
a12 = Exp[-I * k2[E1, Ub, m2] * x2];
a15 = Exp[I * k3[E1, V, m3] * x2];
a16 = Exp[-I * k3[E1, V, m3] * x2];


(*Now build the Matrixes: *)
```

$$Ma1 = \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix};$$
$$Ma2 = \begin{pmatrix} a_5 & a_6 \\ a_7 & a_8 \end{pmatrix};$$
$$Ma3 = \begin{pmatrix} a_9 & a_{10} \\ a_{11} & a_{12} \end{pmatrix};$$
$$Ma4 = \begin{pmatrix} a_{13} & a_{14} \\ a_{15} & a_{16} \end{pmatrix};$$

```
Q1 = FullSimplify[Inverse[Ma1].Ma2.Inverse[Ma3].Ma4];
(* NOTE! the following way as use Q1 =FullSimplify[(1/Qa1).Qa2.(1/Qa3).Qa4] is WRONG,
becasue 1/Qa1 is not inversed matrix *)
(* Inverse[Qa1]=
```

$$\left\{\left\{\frac{a6}{-a2\ a5+a1\ a6},-\frac{a2}{-a2\ a5+a1\ a6}\right\},\left\{-\frac{a5}{-a2\ a5+a1\ a6},\frac{a1}{-a2\ a5+a1\ a6}\right\}\right\} \text{ while } 1/Qa1=\left\{\left\{\frac{1}{a1},\frac{1}{a2}\right\},\left\{\frac{1}{a5},\frac{1}{a6}\right\}\right\} \quad *)$$

```
FullSimplify[Q1[[1, 1]]]
```

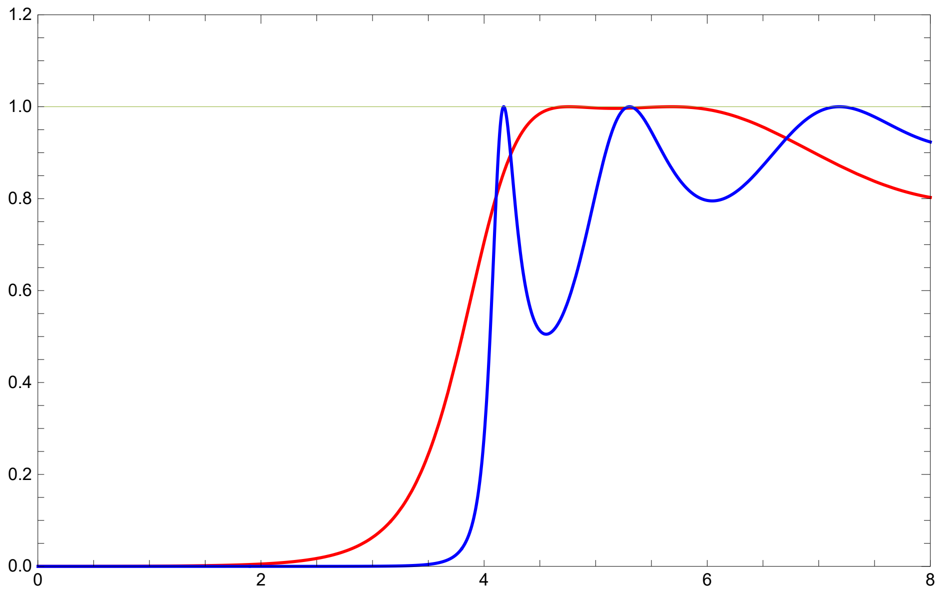
Out[#]=

$$\frac{1}{4\,m2\,m3\,k1[E1,m1]\,k2[E1,Ub,m2]}\,e^{-i\,(x1\,k1[E1,m1]+(x1+x2)\,k2[E1,Ub,m2]-x2\,k3[E1,V,m3])}\left(-e^{2\,i\,x2\,k2[E1,Ub,m2]}\,(m2\,k1[E1,m1]-m1\,k2[E1,Ub,m2])\,(-m3\,k2[E1,Ub,m2]+m2\,k3[E1,V,m3])+e^{2\,i\,x1\,k2[E1,Ub,m2]}\,(m2\,k1[E1,m1]+m1\,k2[E1,Ub,m2])\,(m3\,k2[E1,Ub,m2]+m2\,k3[E1,V,m3])\right)$$

```
In[]:= (*NOW COPY AND PAST THIS Q1[[1,1]] ON THE RIGHT SIDE as
         making the "USER-FUNCTION" M11[E1_,x1_,x2_,Ub_,V_,m1_,m2_,m3_] :*)

Q11[E1_, x1_, x2_, Ub_, V_, m1_, m2_, m3_] :=
   1/(4 m2 m3 k1[E1, m1] k2[E1, Ub, m2]) e^(-i (x1 k1[E1,m1] + (x1+x2) k2[E1,Ub,m2] - x2 k3[E1,V,m3]))
    (-e^(2 i x2 k2[E1,Ub,m2]) (m2 k1[E1, m1] - m1 k2[E1, Ub, m2]) (-m3 k2[E1, Ub, m2] + m2 k3[E1, V, m3]) +
      e^(2 i x1 k2[E1,Ub,m2]) (m2 k1[E1, m1] + m1 k2[E1, Ub, m2]) (m3 k2[E1, Ub, m2] + m2 k3[E1, V, m3]));

(* Transmission with effective masses *)

c = 0.262468;    (* 1/(eV*Angstrom^2) *)
(*
c=(2*m0*eV)/(h*h/4π^2)*10^-20 =  0.262468 per 1 eV  (* 1/Angstrom^2 *)
*)
(*  m = m0 - free electon mass, h - Dirac const. *)

m0 = 1.0;
(*m1=0.8*m0;
m2=1.8*m0;
m3=0.8*m0; *)

L = 10.0 (*units = Angstroms*);
Va = 0.0 (*units = eV*);
UB = 3.8 (*units = eV*);

k1[E1_, m1_] :=  (c * E1 * (m1 / m0)) ^ (1 / 2);   (* 1/Angstrom *)
k2[E1_, Ub_, m2_] := (c * (E1 - Ub) * (m2 / m0)) ^ (1 / 2);      (* 1/Angstrom *)
k3[E1_, V_, m3_] := (c * (E1 + V) * (m3 / m0)) ^ (1 / 2);

Dtransmission[E1_, m1_, m2_, m3_] := Re[m1 / m3 * k3[E1, Va, m3] / k1[E1, m1] *
    1 / (Q11[E1, 0, L, UB, Va, m1, m2, m3] * Conjugate[Q11[E1, 0, L, UB, Va, m1, m2, m3]])]
```

```
m1 = 0.99 * m0;   m12 = 1.0 * m0;
m2 = 0.2 * m0;   m22 = 1.0 * m0;
m3 = 0.99 * m0;   m32 = 1.0 * m0;
Plot[{Dtransmission[E1, m1, m2, m3], Dtransmission[E1, m12, m22, m32], 1}, {E1, 0, 8},
 PlotRange → {{0, 8.0}, {0, 1.2}}, Frame → True, PlotStyle → {Red, Blue, Thin}]
(*RESULT*)
```

Out[ ]=



In[ ]:=