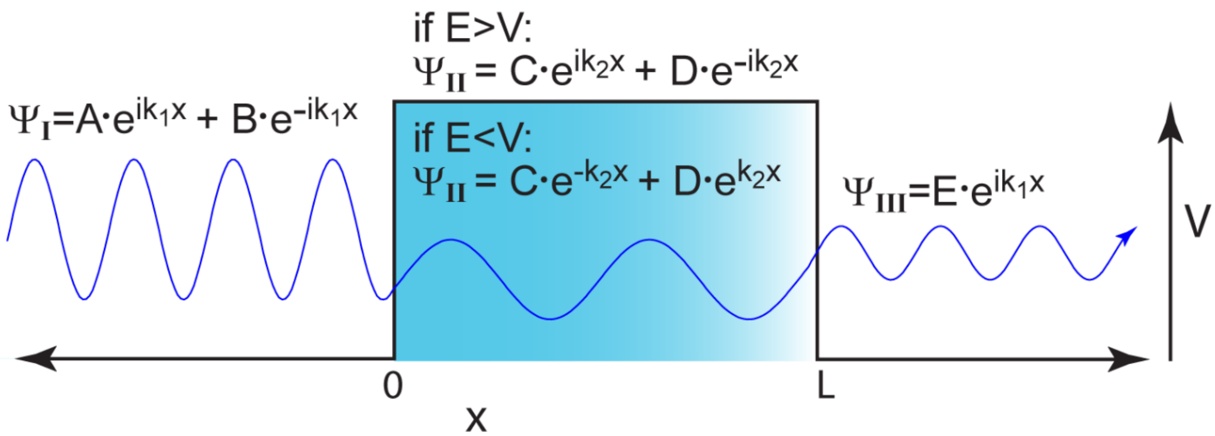
Solution to the Finite Barrier Problem

The finite barrier problem helps us understand that a particle can pass though a barrier that it doesn't have enough energy to pass through. Likewise, sometimes the particle will "bounce back" from hitting a barrier even if it has enough energy to overcome it.

The potential surface is as follows:



It must be noted that the general solution to the wavefunction in the middle barrier depends on whether the energy is greater or less than the potential energy. If E<V, then $k_2 = \sqrt{2m(E-V)}/\hbar^2 = \sqrt{-2m(V-E)}/\hbar^2 = i\sqrt{2m(V-E)}/\hbar^2$ since E-V is negative in this case. As a result, the "general solution" wavefunction that is applicable if E>V:

$$\psi_{II} = Ce^{ik_2x} + De^{-ik_2x}$$

becomes: $\psi_{II} = Ce^{-k_2x} + De^{k_2x}$ when E<V. Thus, we have to solve the transmission probability as a function of whether the energy is greater or less than the potential energy.

In region I, the incoming "A" wave can reflect after hitting a wall to create a "B" wave:

$$\psi_I = Ae^{ik_1x} + Be^{-ik_1x}$$

However, in region III, if the particle passes through the barrier it will travel to the right forever, so there is no need to have any wave except a right-moving "E" wave:

$\psi_{III} = Ee^{ik_1x}$. Note that the momentum k_1 is the same as in region I.

Transmission, E<V

@X=0

Continuous (the wavefunctions are equal):

$$Ae^{ik_1x} + Be^{-ik_1x} = Ce^{-k_2x} + De^{k_2x}$$

Since x=0:

$$A + B = C + D \qquad \textbf{(1)}$$

Smooth (the derivatives are equal):

$$ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x} = -k_2Ce^{-k_2x} + k_2De^{k_2x}$$

Since x=0:

$$ik_1A - ik_1B = -k_2C + k_2D \qquad \textbf{(2)}$$

Now the strategy is to define A in terms of C and D by eliminating B:

since $B = C + D - A$, insert this into (2):

simplification

$$ik_1A - ik_1(C + D - A\,) = -k_2C + k_2D$$

$$ik_1A - ik_1C - ik_1D + ik_1A \; = -k_2C + k_2D$$

$$2ik_1A = -k_2C + k_2D + ik_1C + ik_1D$$

$$2ik_1A = -C(k_2 + ik_1) + D(k_2 - ik_1) \qquad \textbf{(3)}$$

Now we just have to define C and D in terms of E to determine $\frac{E}{A}$. To do this we have to look at the x=L side.

@X=L

Continuous (the wavefunctions are equal):

$$Ce^{-k_2L} + De^{k_2L} = Ee^{ik_1L}$$

Now we will solve for C in terms of E by eliminating D:

$De^{k_2L} = Ee^{ik_1L} - Ce^{-k_2L}$ and by multiplying by e^{-k_2L}:

$$D = Ee^{ik_1L}e^{-k_2L} - Ce^{-2k_2L} \qquad \textbf{(4)}$$

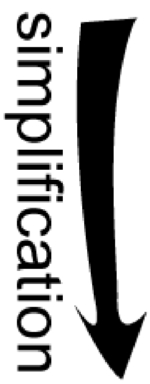
Smooth (the derivatives are equal):

$$-k_2Ce^{-k_2L} + k_2De^{k_2L} = ik_1Ee^{ik_1L} \quad \textbf{(5)}$$

Insert (4) into (5):

$$-k_2Ce^{-k_2L} + k_2\left(Ee^{ik_1L}e^{-k_2L} - Ce^{-2k_2L}\right)e^{k_2L} = ik_1Ee^{ik_1L}$$

Now just do a lot of factoring to get C in terms of E:



$$-k_2Ce^{-k_2L} + k_2Ee^{ik_1L}e^{k_2L}e^{-k_2L} - k_2Ce^{-2k_2L}e^{k_2L} = ik_1Ee^{ik_1L}$$

$$-k_2Ce^{-k_2L} - k_2Ce^{-k_2L} = -k_2Ee^{ik_1L} + ik_1Ee^{ik_1L}$$

$$-2k_2Ce^{-k_2L} = -Ee^{ik_1L}(k_2 - ik_1)$$

$$C = -E\frac{e^{ik_1L}(k_2-ik_1)}{-2k_2e^{-k_2L}}$$

$$C = E\frac{e^{ik_1L}(k_2-ik_1)}{2k_2e^{-k_2L}} \quad \textbf{(6)}$$

Done! Now we have to start over to solve D in terms of E.

Continuous (the wavefunctions are equal):

$$Ce^{-k_2L} + De^{k_2L} = Ee^{ik_1L}$$

Now we will solve for D in terms of E by eliminating C:

$Ce^{-k_2L} = Ee^{ik_1L} - De^{k_2L}$ and by multiplying by e^{k_2L}:

$$C = Ee^{ik_1L}e^{k_2L} - De^{2k_2L} \quad \textbf{(7)}$$

Now we can insert eq. (6) into (7), but instead I will do this in a more analogous manner as above because I am comfortable with this route at this point.

Using the fact that the equations are smooth (the derivatives are equal):

$$-k_2Ce^{-k_2L} + k_2De^{k_2L} = ik_1Ee^{ik_1L} \quad \textbf{(5)}$$

Insert (7) into (5):

$$-k_2\left(Ee^{ik_1L}e^{k_2L} - De^{2k_2L}\right)e^{-k_2L} + k_2De^{k_2L} = ik_1Ee^{ik_1L}$$

Now just do a lot of factoring to get D in terms of E:

$$-Ek_2e^{ik_1L}e^{k_2L}e^{-k_2L} + Dk_2e^{2k_2L}e^{-k_2L} + k_2De^{k_2L} = ik_1Ee^{ik_1L}$$

$$k_2De^{k_2L} + k_2De^{k_2L} = ik_1Ee^{ik_1L} + k_2Ee^{ik_1L} = Ee^{ik_1L}(k_2 + ik_1)$$

$$D = E\frac{e^{ik_1L}(k_2+ik_1)}{2k_2e^{k_2L}}$$ **(8)**

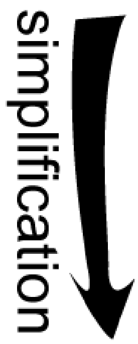
Now we are going to take equation (3):

$$2ik_1A = -C(k_2 + ik_1) + D(k_2 - ik_1)$$

And plug in eq. (6) for $C = E\frac{e^{ik_1L}(k_2-ik_1)}{2k_2e^{-k_2L}}$ and (8) for $D = E\frac{e^{ik_1L}(k_2+ik_1)}{2k_2e^{k_2L}}$:

$$2ik_1A = -E\frac{e^{ik_1L}(k_2-ik_1)}{2k_2e^{-k_2L}}(k_2 + ik_1) + E\frac{e^{ik_1L}(k_2+ik_1)}{2k_2e^{k_2L}}(k_2 - ik_1)$$

Now we just try to simplify and factor variables out the wazoo:



$$2ik_1A = E\left(-\frac{e^{ik_1L}(k_2-ik_1)}{2ik_12k_2e^{-k_2L}}(k_2 - ik_1) + \frac{e^{ik_1L}(k_2+ik_1)}{2ik_12k_2e^{k_2L}}(k_2 + ik_1)\right)$$

$$2ik_1A = E\left(-\frac{e^{ik_1L}(k_2-ik_1)^2}{2k_2e^{-k_2L}} + \frac{e^{ik_1L}(k_2+ik_1)^2}{2k_2e^{k_2L}}\right)$$

$$2ik_1A = E\frac{e^{ik_1L}}{2k_2}\left(e^{-k_2L}(k_2 + ik_1)^2 - e^{k_2L}(k_2 - ik_1)^2\right)$$

$$\frac{E}{A} = \frac{2ik_1}{\frac{e^{ik_1L}}{2k_2}\left(e^{-k_2L}(k_2+ik_1)^2 - e^{k_2L}(k_2-ik_1)^2\right)}$$

Here is about as far as I can take it in terms of factoring:

$$\frac{E}{A} = \frac{4ik_1k_2e^{-ik_1L}}{e^{-k_2L}(k_2+ik_1)^2 - e^{k_2L}(k_2-ik_1)^2}$$ **(9)**

Transmission, E>V

@X=0

Continuous (the wavefunctions are equal):

$$Ae^{ik_1x} + Be^{-ik_1x} = Ce^{ik_2x} + De^{-ik_2x}$$

Since x=0:

$$A + B = C + D \qquad \textbf{(1)}$$

Smooth (the derivatives are equal):

$$ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x} = ik_2Ce^{ik_2x} - ik_2De^{-ik_2x}$$

Since x=0:

$ik_1A - ik_1B = ik_2C - ik_2D$ Note we can eliminate all the i's:

$$k_1A - k_1B = k_2C - k_2D \qquad \textbf{(2)}$$

Now the strategy is to define A in terms of C and D by eliminating B:

since $B = C + D - A$, which we insert into (2):

simplification ↓

$$k_1A - k_1(C + D - A) = k_2C - k_2D$$

$$k_1A - k_1C - k_1D + k_1A = k_2C - k_2D$$

$$2k_1A = k_2C - k_2D + k_1C + k_1D$$

$$2k_1A = C(k_2 + k_1) - D(k_2 - k_1) \qquad \textbf{(3)}$$

Now we just have to define C and D in terms of E to determine $\frac{E}{A}$. To do this we have to look at the x=L side.

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Now we will solve for C in terms of E by eliminating D:

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$$k_2 C e^{ik_2 L} - k_2 D e^{-ik_2 L} = k_1 E e^{ik_1 L} \qquad \textbf{(5)}$$

Insert (4) into (5):

$$k_2 C e^{ik_2 L} - k_2 \left(E e^{ik_1 L} e^{ik_2 L} - C e^{2ik_2 L}\right) e^{-ik_2 L} = k_1 E e^{ik_1 L}$$

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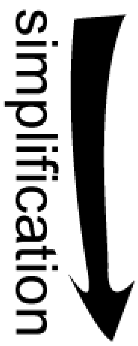

$$k_2 C e^{ik_2 L} - k_2 \left(E e^{ik_1 L} e^{ik_2 L} - C e^{2ik_2 L}\right) e^{-ik_2 L} = k_1 E e^{ik_1 L}$$

$$k_2 C e^{ik_2 L} - k_2 E e^{ik_1 L} e^{ik_2 L} e^{-ik_2 L} + k_2 C e^{2ik_2 L} e^{-ik_2 L} = k_1 E e^{ik_1 L}$$

$$k_2 C e^{ik_2 L} + k_2 C e^{ik_2 L} = k_1 E e^{ik_1 L} + k_2 E e^{ik_1 L}$$

$$2k_2 C e^{ik_2 L} = E e^{ik_1 L}(k_1 + k_2)$$

$$C = E \frac{e^{ik_1 L}(k_1 + k_2)}{2k_2 e^{ik_2 L}} \qquad \textbf{(6)}$$

Done! Now we have to start over to solve D in terms of E.

Continuous (the wavefunctions are equal):

$$C e^{ik_2 L} + D e^{-ik_2 L} = E e^{ik_1 L}$$

Now we will solve for D in terms of E by eliminating C:

$C e^{ik_2 L} = E e^{ik_1 L} - D e^{-ik_2 L}$ and by multiplying by $e^{-ik_2 L}$:

$$C = E e^{ik_1 L} e^{-ik_2 L} - D e^{-ik_2 L} e^{-ik_2 L} = E e^{i(k_1 - k_2)L} - D e^{-2ik_2 L} \qquad \textbf{(7)}$$

Now we can insert eq. (6) into (7), but instead I will do this in a more analogous manner as above because I am comfortable with this route at this point.

Using the fact that the equations are smooth (the derivatives are equal):

$$k_2 C e^{ik_2 L} - k_2 D e^{-ik_2 L} = k_1 E e^{ik_1 L} \qquad \textbf{(5)}$$

Insert (7) into (5):

$$k_2 \left(E e^{i(k_1 - k_2)L} - D e^{-2ik_2 L}\right) e^{ik_2 L} - k_2 D e^{-ik_2 L} = k_1 E e^{ik_1 L}$$

Now just do a lot of factoring to get D in terms of E:

simplification ↓

$$k_2Ee^{i(k_1-k_2)L}e^{ik_2L} - k_2De^{-2ik_2L}e^{ik_2L} - k_2De^{-ik_2L} = k_1Ee^{ik_1L}$$

$$k_2De^{-ik_2L} + k_2De^{-ik_2L} = -k_1Ee^{ik_1L} + k_2Ee^{ik_1L}$$

$$2k_2De^{-ik_2L} = Ee^{ik_1L}(k_2 - k_1)$$

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Now we are going to take equation (3):

$$2k_1A = C(k_2 + k_1) - D(k_2 - k_1)$$

And plug in eq. (6) for $C = E\frac{e^{ik_1L}(k_1+k_2)}{2k_2e^{ik_2L}}$ and (8) for $D = E\frac{e^{ik_1L}(k_2-k_1)}{2k_2e^{-ik_2L}}$:

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Now we just try to simplify and factor variables out the wazoo:

simplification ↓

$$2k_1A = E\frac{e^{ik_1L}(k_1+k_2)}{2k_2e^{ik_2L}}(k_2 + k_1) - E\frac{e^{ik_1L}(k_2-k_1)}{2k_2e^{-ik_2L}}(k_2 - k_1)$$

$$2k_1A = E\frac{e^{ik_1L}}{2k_2}\left(e^{-ik_2L}(k_1 + k_2)^2 - e^{ik_2L}(k_2 - k_1)^2\right)$$

$$\frac{E}{A} = \frac{2k_1}{\frac{e^{ik_1L}}{2k_2}\left(e^{-ik_2L}(k_1+k_2)^2 - e^{ik_2L}(k_2-k_1)^2\right)}$$

Here is about as far as I can take it in terms of factoring:

$$\frac{E}{A} = \frac{4k_1k_2e^{-ik_1L}}{\left(e^{-ik_2L}(k_1+k_2)^2 - e^{ik_2L}(k_2-k_1)^2\right)} \qquad \textbf{(9)}$$

On the next page we will fit these results (the %T as a function of energy above and below the barrier) together in a graph.

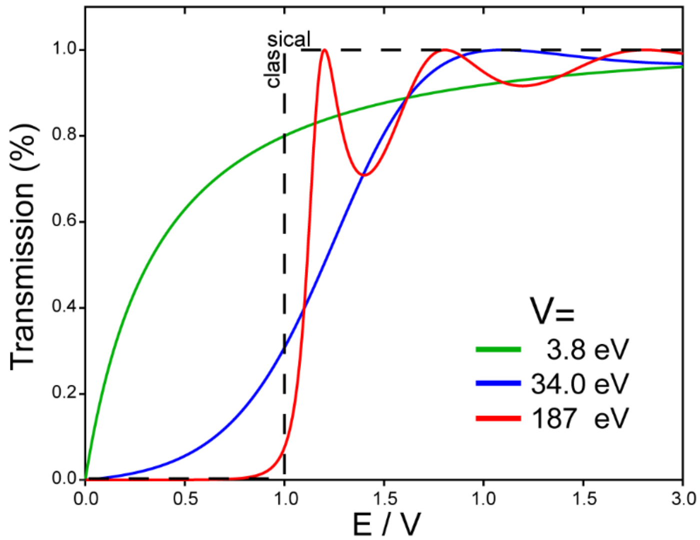
Results!

Now we take the two equations for the %T, where energy is below and above the potential energy barrier, and plot them together using Matlab. To simulate a real particle the following parameters were used:

mass = an electron = $9.109{\times}10^{-31}$ kg, Length = 1 nm = $1{\times}10^{-9}$ m

So this is an electron hitting a ~1 nm barrier. Note that the classical %T is just 0 if the particle's energy is below the barrier and 100% if it has more energy than the barrier (dotted line). However, we can see via $\frac{|E|^2}{|A|^2}$ that quantum mechanics stipulates that there is a finite chance of passing through the barrier even though the particle doesn't have enough energy to do so!

Note that the %T is shown for three barriers of increasing strength. Notice how, in the case of a large barrier (red line), that increasing the energy varies from "helping" the electron cross the barrier, then minimizes, and then increases the %T a few times as the particle has greater kinetic energy.



Here are 3-D plots that represent the same: