The Finite Square Well

Scattering state

\((E > U_0)\)

\[ U(x) = \begin{cases} 
0 & |x| < L/2 \\
U_0 & |x| \geq L/2 
\end{cases} \] \hfill (1)

where \(U_0\) is a positive constant.
Solution for $x < -L/2$

In the region $x < -L/2$

$$-rac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U_0 \psi = E \psi \quad (2)$$

or

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m(E - U_0)}{\hbar^2} \psi = 0 \quad (3)$$

Since $E > U_0$, define

$$k = \sqrt{\frac{2m(E - U_0)}{\hbar^2}} \quad (4)$$

Eq.(3) becomes

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad (5)$$

Solution of Eq.(5) is

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad (6)$$

Here both $e^{ikx}$ and $e^{-ikx}$ are finite even if $x \to -\infty$ and should be retained.
Solution for $x > L/2$

Similarly, in the region $x > L/2$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U_0 \psi = E\psi$$  \hspace{1cm} (7)

or

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0$$  \hspace{1cm} (8)

where

$$k = \sqrt{\frac{2m(E - U_0)}{\hbar^2}}$$  \hspace{1cm} (9)

Solution of Eq. (8) is

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}$$  \hspace{1cm} (10)

Here both $e^{ikx}$ and $e^{-ikx}$ are finite even if $x \to \infty$ and should be retained.
Solution for $-L/2 < x < L/2$

Finally in the region $-L/2 < x < L/2$, $U(x) = 0$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi$$  \hspace{1cm} (11)

or

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0$$  \hspace{1cm} (12)

Let

$$k' = \sqrt{\frac{2mE}{\hbar^2}}$$  \hspace{1cm} (13)

Eq.(12) becomes

$$\frac{\partial^2 \psi}{\partial x^2} + k'^2 \psi = 0$$  \hspace{1cm} (14)

Solution of Eq.(14) is

$$\psi(x) = Ce^{ik'x} + De^{-ik'x}$$  \hspace{1cm} (15)
General Solution

Equations (6), (10) and (15) are the general solutions of the Schrödinger equation in the three regions respectively. The parameters $A$, $B$, $C$, $D$, $F$ and $G$, plus the energy of the particle, are determined in principle by the boundary conditions (4 equations) and the normalization of the wave function.

You may realize that there are more unknowns than equations. This is very typical for the so-called scattering states.

Note that in each region, $e^{ikx}$ or $e^{ikx-\omega t} = e^{ipx/\hbar-Et/\hbar}$ represents a wave traveling along the $+x$ direction, where $e^{-ikx}$ represent a wave traveling along the $-x$ direction.

Relative to the quantum well region, $e^{ikx}$ represents an incoming or wave, $e^{-ikx}$ represent an outgoing wave in the region $x < -L/2$. For $x > L/2$, $e^{ikx}$ is an outgoing wave and $e^{-ikx}$ is the incoming wave.
Scattering States

A better defined problem could be as the following: a wave is incident from the left of the quantum well, part of the wave is reflected and part is transmitted through the quantum well.

\[
\psi(x) = \begin{cases} 
  Ae^{ikx} + Be^{-ikx} & x \leq -L/2 \\
  Ce^{ik'x} + De^{-ik'x} & -L/2 < x < L/2 \\
  Fe^{iL/2} & x > L/2 
\end{cases}
\]

(16)
Scattering States

In a typical scattering problem, particles with known energy are fired in from one direction (from left in this case → no incident wave on the right side of the well), and we are more interested in the region far away from the scattering centre (quantum well in this case).

On the left side of the well, $A e^{ikx}$ is the **incident wave** and $A$ is its amplitude, $B e^{-ikx}$ is the **reflected wave** and $B$ is its amplitude. To the right side of the well, $F e^{ikx}$ is the **transmitted wave** and $F$ is its amplitude.

For a wave $\phi = A e^{ikx}$, the corresponding probability current density is given by

$$J = \frac{i\hbar}{2m} \left( \phi \frac{d\phi^*}{dx} - \phi^* \frac{d\phi}{dx} \right)$$

$$= \frac{i\hbar}{2m} \left( A e^{ikx} \frac{d}{dx} A^* e^{-ikx} - A^* e^{-ikx} \frac{d}{dx} A e^{ikx} \right)$$

$$= \frac{\hbar k}{m} |A|^2$$
Scattering States

Thus the probability current densities corresponding the incident wave, the reflected wave and the transmitted wave are

\[ J_0 = \frac{\hbar k}{m} |A|^2 \]

\[ J_r = \frac{\hbar k}{m} |B|^2 \]

\[ J_t = \frac{\hbar k}{m} |F|^2 \]

The reflection coefficient and transmission coefficinet are defined as

\[ R = \frac{J_r}{J_0} = \frac{|B|^2}{|A|^2} \]

\[ T = \frac{J_t}{J_0} = \frac{|F|^2}{|A|^2} \]
Boundary Conditions

We now determine the reflection and transmission coefficients using the boundary conditions.

At $x = L/2$

$$Ce^{ik'L/2} + De^{-ik'L/2} = Fe^{ikL/2}$$

$$ik' \left( Ce^{ik'L/2} - De^{-ik'L/2} \right) = ikFe^{ikL/2}$$

At $x = -L/2$

$$Ae^{-ikL/2} + Be^{ikL/2} = Ce^{-ik'L/2} + De^{ik'L/2}$$

$$ik \left( Ae^{-ikL/2} - Be^{ikL/2} \right) = ik' \left( Ce^{-ik'L/2} - De^{ik'L/2} \right)$$

Two of the above equations can be used to eliminate $C$ and $D$, the remaining two can be used to solve $B$ and $F$ in terms of $A$ (see following pages).
Boundary Conditions

Eliminate $D$ using the first two equations on the last page,

$$2k'C e^{ik'L/2} = (k' + k)F e^{ikL/2}$$  \hspace{1cm} (17)

Eliminate $D$ using the last two equations on the last page,

$$2k'C e^{-ik'L/2} = (k' + k)A e^{-ikL/2} + (k' - k)B e^{ikL/2}$$  \hspace{1cm} (18)

Divide these two equations

$$e^{-ik'L} = \frac{A}{F} e^{-ikL} + \left(\frac{k' - k}{k' + k}\right) \frac{B}{F}$$  \hspace{1cm} (19)

Eliminate $C'$ using the first two equations on the last page

$$2k'D e^{-ik'L/2} = (k' - k)F e^{ikL/2}$$  \hspace{1cm} (20)

Eliminate $C'$ using the last two equations on the last page

$$2k'D e^{ikL/2} = (k' - k)A e^{-ikL/2} + (k' + k)B e^{ikL/2}$$  \hspace{1cm} (21)

Divide these two equations

$$e^{ik'L} = \frac{A}{F} e^{-ikL} + \left(\frac{k' + k}{k' - k}\right) \frac{B}{F}$$  \hspace{1cm} (22)
Transmission Coefficient

Now solving $B/F$ from Eqs. (19) and (22) by eliminating $A/F$, we get

$$\frac{B}{F} = \frac{i(k'^2 - k^2) \sin(k'L)}{2kk'}$$  \hspace{1cm} (23)

Next solve $A/F$ from Eqs. (19) and (22) by eliminating $B/F$, we get

$$\frac{F}{A} = \frac{2kk' e^{-ikL}}{2kk' \cos(k'L) - i(k'^2 + k^2) \sin(k'L)}$$  \hspace{1cm} (24)

Transmission coefficient

$$T = \left| \frac{F}{A} \right|^2$$

$$\frac{1}{T} = 1 + \frac{(k'^2 - k^2)^2 \sin^2(k'L)}{4k^2 k'^2}$$
Transmission Coefficient

Replace $k$ and $k'$ by expressions given in Eqs. (9) and (13)

$$
\frac{1}{T} = 1 + \frac{U_0^2}{4E(E - U_0)} \sin^2 \left( \sqrt{\frac{2mL^2E}{\hbar^2}} \right)
$$

(25)

Graph of $T$ vs. $E/E_0$ where $E_0 = \hbar^2/(2mL^2)$.

$U_0$ is set to $200E_0$ in the above figure.

Please change the value of $U_0$ in excel file lec12.xls and observe change in the graph.
Reflection Coefficient

Reflection coefficient:

\[ R = \left| \frac{B}{A} \right|^2 = \left| \frac{B}{F} \right|^2 \left| \frac{F}{A} \right|^2 = \frac{(k'^2 - k^2)^2 \sin^2(k'L)}{4k'^2k'^2} T \]

or

\[ R = \frac{U_0^2 \sin^2(\sqrt{E/E_0})}{4E(E - U_0)} T \]

Note that

\[ T + R = \left[ 1 + \frac{U_0^2 \sin^2(\sqrt{E/E_0})}{4E(E - U_0)} \right] T = 1 \]

Particles are either reflected and/or transmitted.