Quantum Physics 1
2022

Class 13 – The Step Barrier and Scattering

TISE reminder

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

Piecewise potentials 1 reminder

Solution to the TISE in a region where V is a constant and E>V:

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

Guess: $\psi = e^{ikx}$

$$-\frac{\hbar^2 k^2}{2m} = (E - V) \quad \Rightarrow \quad k = \pm\sqrt{\frac{2m(E - V)}{\hbar^2}}$$

$$\psi = Ae^{ikx} + Be^{-ikx}$$

Piecewise potentials 2 reminder

Solution to the TISE in a region where V is a constant and E<V:

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} - |E-V|\psi(x) = 0$$

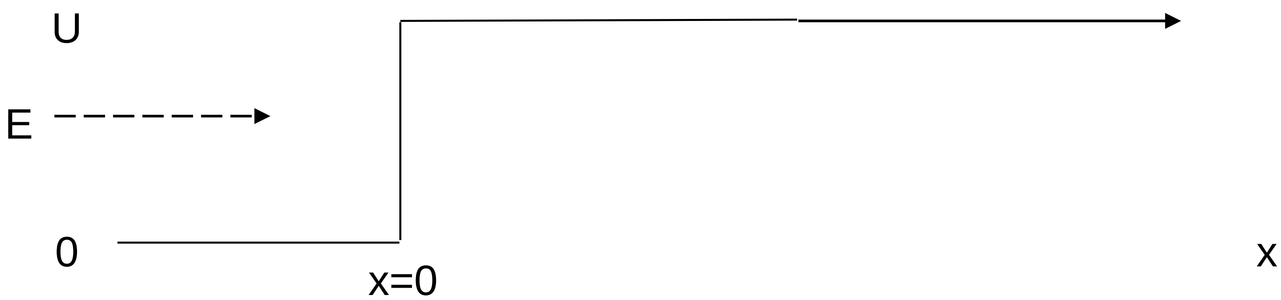
Guess: $\psi = e^{ikx}$

$$\frac{\hbar^2 k^2}{2m} = -|E-V| \quad \Rightarrow \quad k = \pm i\sqrt{\frac{2m|E-V|}{\hbar^2}}$$

Let $K = ik = \pm\sqrt{\frac{2m|E-V|}{\hbar^2}}$ (∴ K is a real number)

$\psi = Ae^{Kx} + Be^{-Kx}$ (exponential growth or decay)

The Step Potential



- State general solutions in each region.
- Carefully eliminate non-physical possibilities.
- Match wavefunctions the boundary.
  - Two possibilities E>V and E<V.

We will work this case together on the worksheet

An example

- Let’s consider the situation where a wave is incident from the left onto a barrier at x=0.
- The wavefunction for pure momentum wave moving left is:

$$\Psi(x,t) = Ae^{ikx-i\omega t}$$

- What can the wave do?
  - It can bounce back, going the other way.

    $$\Psi(x,t) = Be^{-ikx-i\omega t}$$

  - It can pass through the boundary.

    $$\Psi(x,t) = Ce^{ikx-i\omega t}$$

Solutions in two regions

$$\psi_1(x,t) = (Ae^{ik_1x} + Be^{-ik_1x})$$

$$\psi_2(x,t) = Ce^{ik_2x}$$

1) $A + B = C$ (continuity)

2) $ik_1A - ik_1B = ik_2C$ ("smoothity")

$$B = C - A \quad \Rightarrow \quad i2k_1A = i(k_2 + k_1)C \quad \Rightarrow \quad C = \frac{2k_1}{k_2 + k_1}A$$

$$B = \frac{k_1 - k_2}{k_2 + k_1}A$$

In terms of energy: $\dfrac{C}{A} = \dfrac{2\sqrt{2mE/\hbar^2}}{\sqrt{2mE/\hbar^2} + \sqrt{2m(E-V)/\hbar^2}} = \dfrac{2\sqrt{E}}{\sqrt{E} + \sqrt{(E-V)}}$

For E>>V, C/A $\Rightarrow$ 1. For E=V, C/A $\Rightarrow$ 2

Probability current in two regions

$$j(x,t) = \frac{-i\hbar}{2m}\left(\Psi^* \frac{\partial}{\partial x}\Psi - \Psi \frac{\partial}{\partial x}\Psi^*\right)$$

which for a pure momentum state is: $j = k\Psi^*\Psi$

$$j_{incident} = +\frac{\hbar k_1}{m}A^2$$

$$j_{reflected} = -\frac{\hbar k_1}{m}B^2$$

$$j_{transmitted} = +\frac{\hbar k_2}{m}C^2$$

$$T \equiv \frac{j_{transmitted}}{j_{incident}} = \frac{k_2 C^2}{k_1 A^2} = \frac{k_2}{k_1}\left(\frac{2k_1}{k_2 + k_1}\right)^2 = \frac{4k_1 k_2}{(k_2 + k_1)^2}$$

and for E<V

1) $A + B = C$ (continuity)

2) $ik_1 A - ik_1 B = -KC$ ("smoothity")

$B = C - A \quad \Rightarrow \quad i2k_1 A = (-K + ik_1)C \quad \Rightarrow \quad C = \frac{2k_1}{-K + ik_1} A$

$B = \frac{ik_1 + K}{ik_1 - K} A$

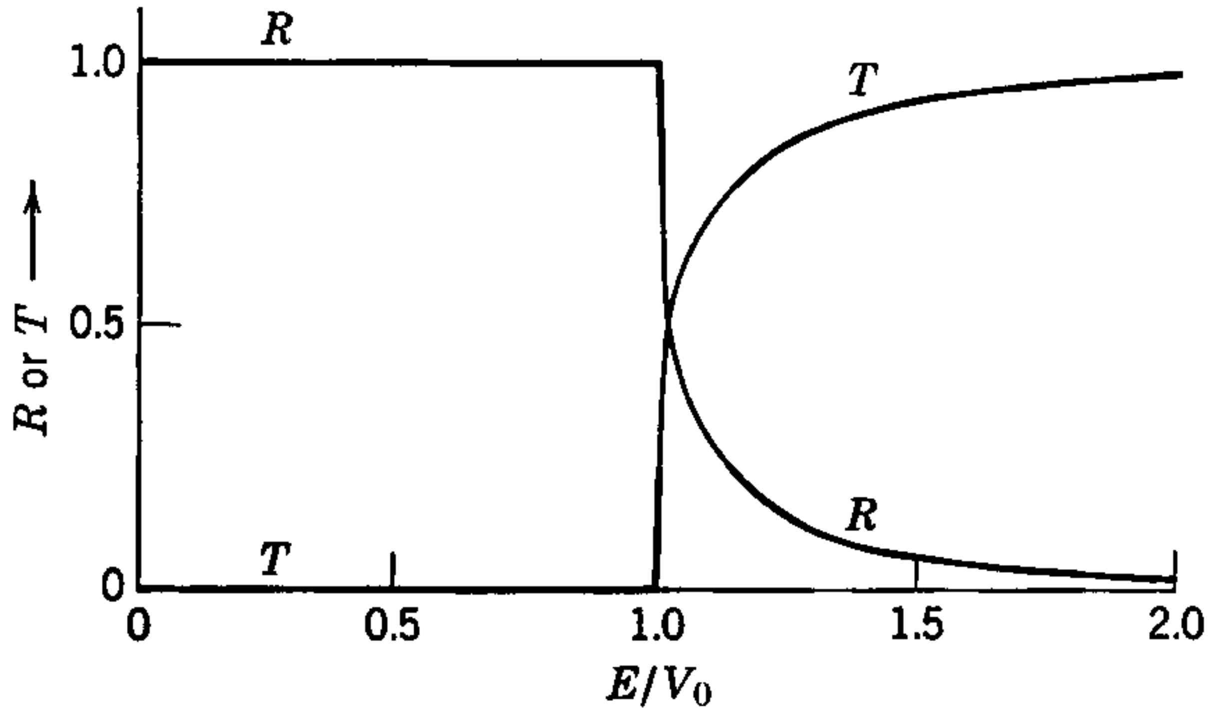
$$j_{incident} = +\frac{\hbar k_1}{m} A^2$$

$$j_{reflected} = -\frac{\hbar k_1}{m} B^2 = -\frac{\hbar k_1}{m} A^2$$

$$j_{transmitted} = \frac{-i\hbar}{2m}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right] = 0$$

$$T \equiv \frac{j_{transmitted}}{j_{incident}} = \frac{k_2 C^2}{k_1 A^2} = \frac{k_2}{k_1}\left(\frac{2k_1}{k_2 + k_1}\right)^2 = \frac{2k_1 k_2}{(k_2 + k_1)^2}$$

$$R = 1$$



R = 1 for $E/V_o < 1$

For $E/V_o > 1$

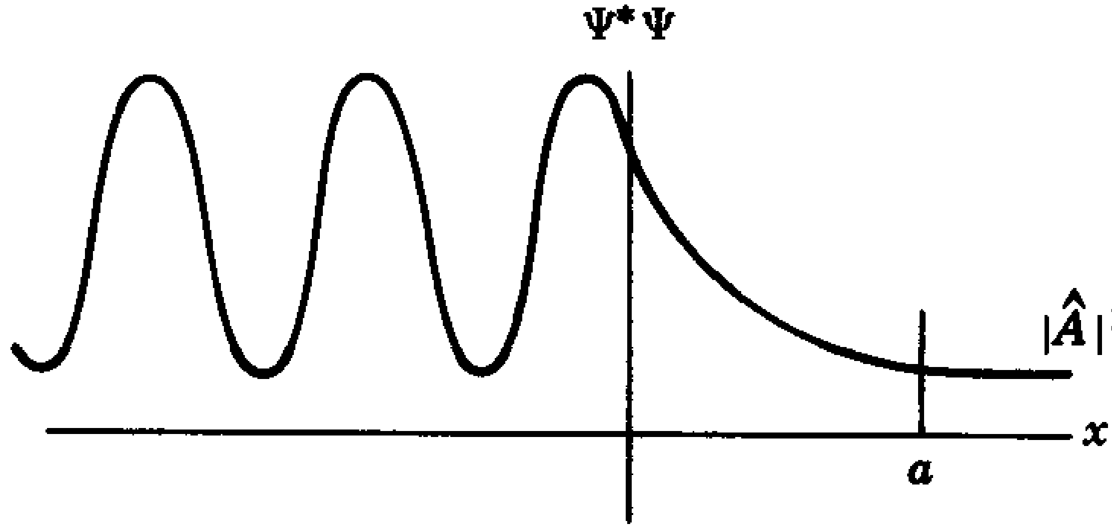
$R = 1 - T$

$$= \left(\frac{1 - \sqrt{1 - \frac{V_o}{E}}}{1 + \sqrt{1 - \frac{V_o}{E}}} \right)^2$$

The reflection and transmission coefficients R and T for a particle incident upon a potential step. The abscissa E/V_0 is the ratio of the total energy of the particle to the increase in its potential energy at the step. The case $k_1 = 2k_2$ corresponds to $E/V_0 = 1.33$.

Figure 5-23

Probability density in a model of barrier penetration.

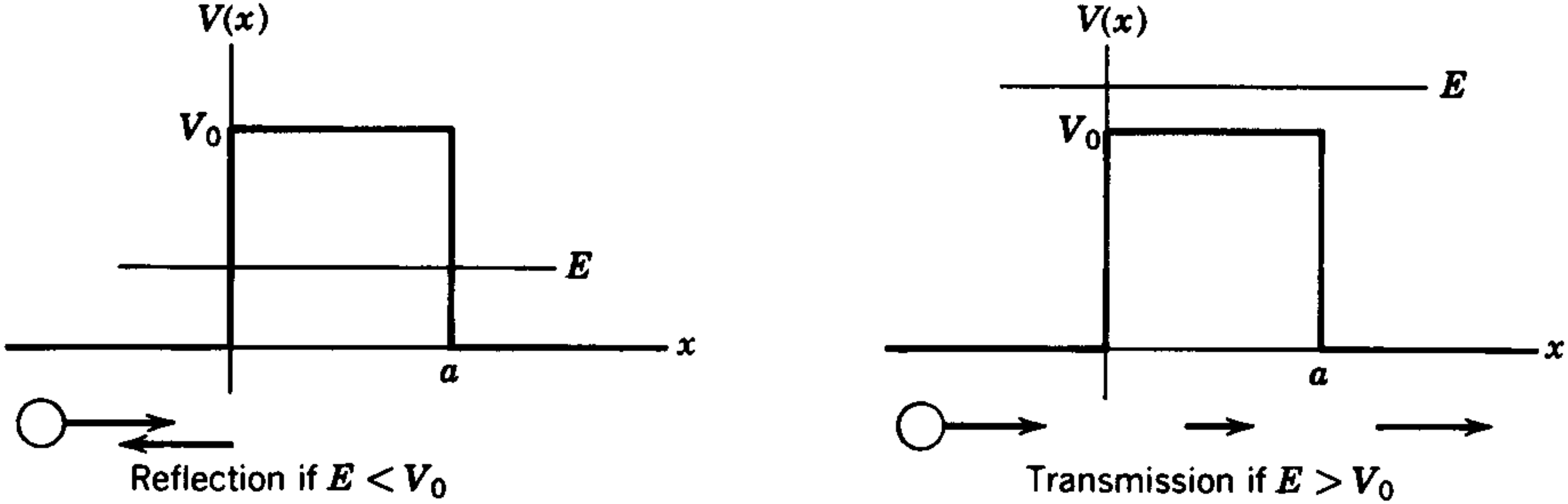


The Step Barrier

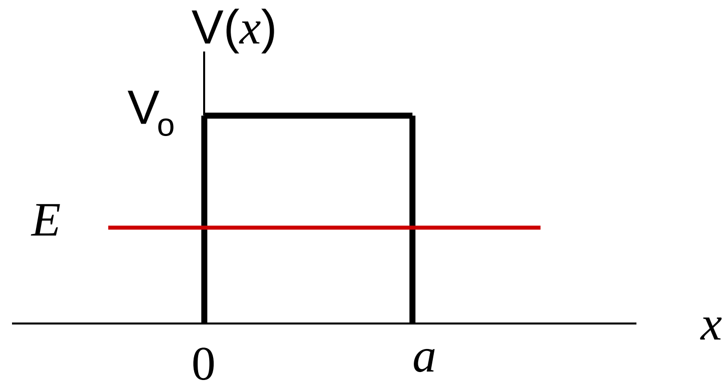
Barrier Potential

$$V(x) = \begin{cases} 0 \; for \; x<0 \; and \; x>a \\ V_0, 0 < x < a \end{cases}$$

Figure 5-21
Reflection and transmission of a classical particle by a rectangular potential energy barrier.



Case 1 $E < V_0$

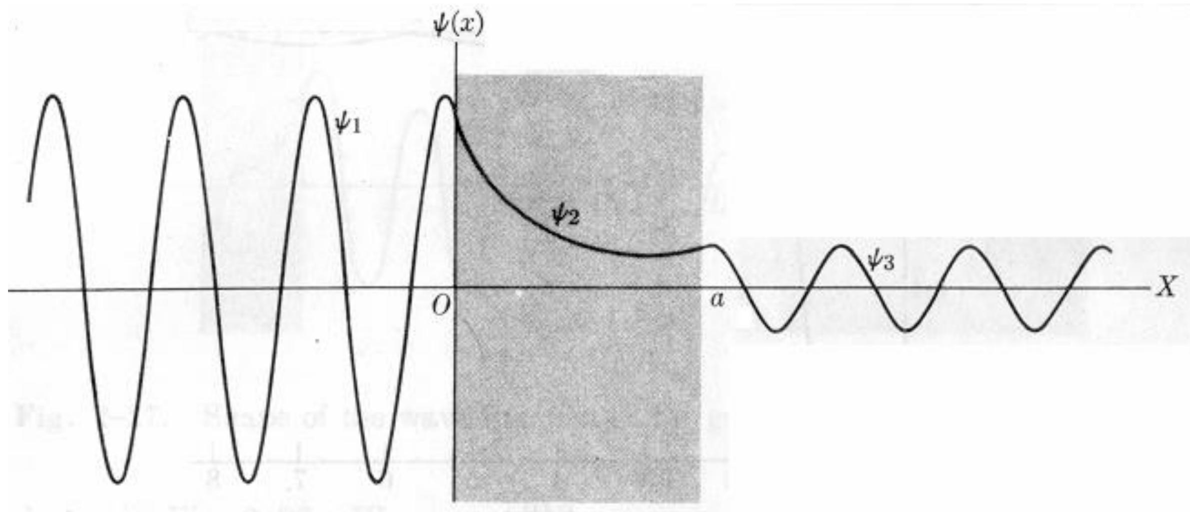


$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1} & x < 0 \\ Ce^{-k_2x} + De^{k_2x} & 0 < x < a \\ \hat{A}e^{ik_1x} + \hat{B}e^{-ik_1x} & x > a \end{cases} \quad (5\text{-}73)$$

where

$$\begin{cases} k_1 = \dfrac{\sqrt{2mE}}{\hbar} \\ k_2 = \dfrac{\sqrt{2m(V_0 - E)}}{\hbar} \end{cases}$$

We expect a wavefunction that looks like this



Use $\hat{B} = 0$ for $x > a$

$$\left.\begin{array}{ll} \psi(o) & \text{continuous} \\ \psi'(o) & \quad '' \end{array}\right\} \text{ at } x = 0$$

$$\left.\begin{array}{ll} \psi(a) & \text{continuous} \\ \psi'(a) & \quad '' \end{array}\right\} \text{ at } x = a$$

Express $B, C, D, \hat{A}$ in terms of A.

$$x = 0$$

$\psi(x)$: $\quad Ae^{ik_1x} + Be^{-ik_1x} \quad\quad Ce^{-k_2x} + De^{k_2x}$

$\psi(0)$: $\quad A + B \quad = C + D$ (1)

$\psi'(x)$: $\quad ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x} \quad\quad -k_2Ce^{-k_2x} + k_2De^{k_2x}$

$\psi'(0)$: $\quad ik_1(A - B) \quad = -k_2(C - D)$ (2)

$$x = a$$

$\psi(x)$: $\quad Ce^{-k_2x} + De^{k_2x} \quad\quad \hat{A}e^{ik_1x}$

$\psi(a)$: $\quad Ce^{-k_2a} + De^{k_2a} \quad = \hat{A}e^{ik_1a}$ (3)

$\psi'(x)$: $\quad -k_2\left(Ce^{-k_2x} - De^{k_2x}\right) \quad\quad ik_1\hat{A}e^{ik_1x}$

$\psi'(a)$: $\quad -k_2\left(Ce^{-k_2a} - De^{k_2a}\right) \quad = ik_1\hat{A}e^{ik_1a}$ (4)

$$\left|\frac{A}{\hat{A}}\right|^2 = 1 + \frac{1}{4}\left(\frac{k_2}{k_1} + \frac{k_1}{k_2}\right)^2 \sinh k_2\, a$$

$$\left|\frac{B}{\hat{A}}\right|^2 = \frac{1}{4}\left(\frac{k_2}{k_1} + \frac{k_1}{k_2}\right)^2 \sinh k_2\, a$$

Transmission coefficient T

$$T = \left|\frac{\hat{A}}{A}\right|^2 = \frac{1}{1 + \frac{1}{4}\left(\frac{k_2}{k_1} + \frac{k_1}{k_2}\right) \sinh^2 k_2 \quad a} = \frac{1}{1 + \frac{\sinh^2 k_2\, a}{4\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)}}$$

Reflection coefficient R

$$R = \left|\frac{B}{A}\right|^2 = \left|\frac{B}{\hat{A}}\right|^2 \left|\frac{\hat{A}}{A}\right|^2$$

$$= \frac{1}{4}\left(\frac{k_2}{k_1} + \frac{k_1}{k_2}\right)^2 \sinh^2 k_2\, a * \left|\frac{\hat{A}}{A}\right|^2$$

Recall $$T = \left|\frac{\hat{A}}{A}\right|^2 = \frac{1}{1 + \frac{1}{4}\left(\frac{k_2}{k_1} + \frac{k_1}{k_2}\right)^2 \sinh^2 k_2\, a}$$

Note: $T + R = 1$

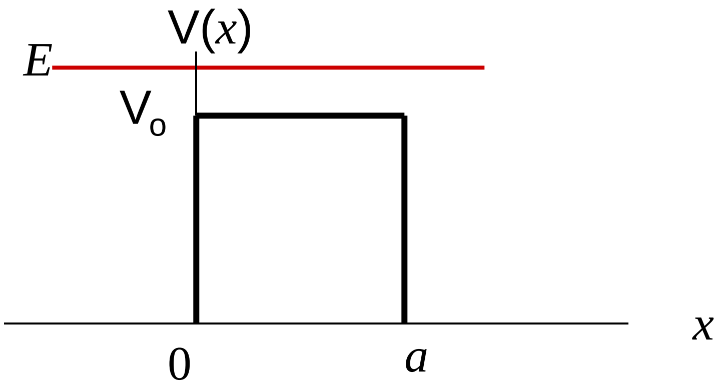
Approximate transmission coefficient when $a \rangle\rangle \frac{1}{k_2}$

$$T = 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2k_2 a}$$

$$\sinh u = \frac{1}{2}\left(e^{u} - e^{-u}\right) \quad and \quad u = k_2 a$$

This form is frequently used as an approximation in tunnelling calculations.
Examples: STM, Quantum wells and barriers in semiconductors, nuclear decay

Case 2 $E > V_0$



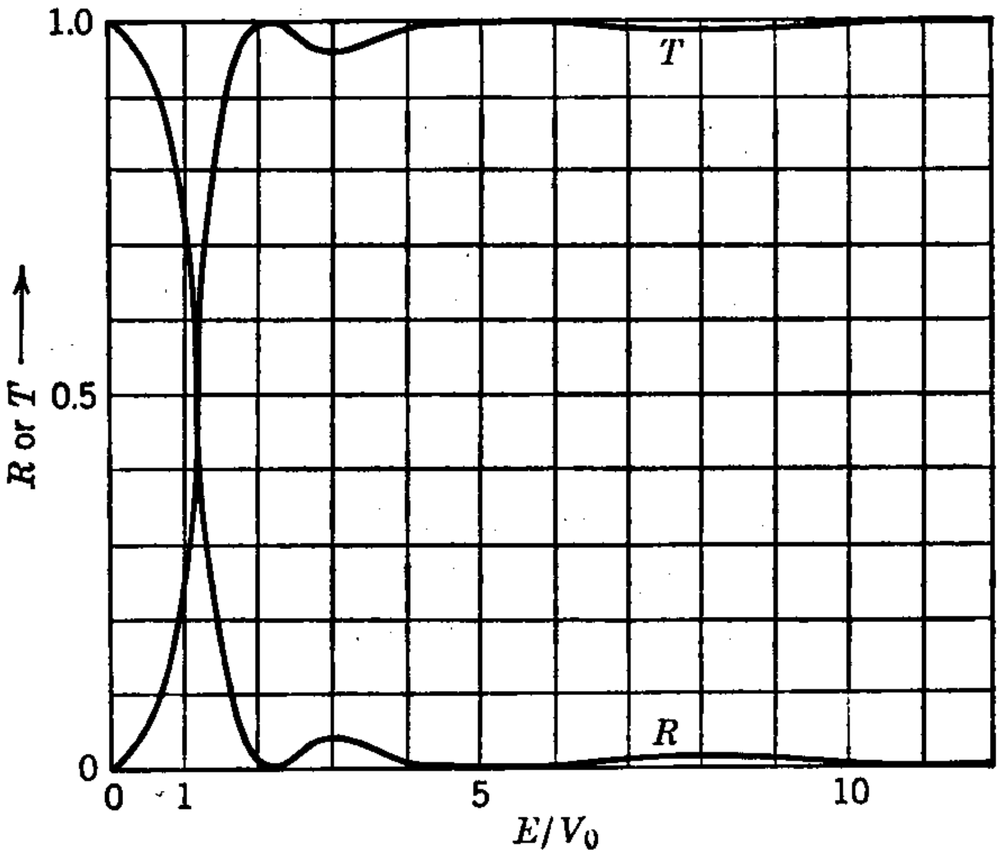
$$\psi(x) = \begin{cases} \hat{A}e^{ik1x}+\hat{B}e^{-ik_1x} & x > a \\ Ae^{ik_1x}+Be^{-ik_1x} & x < 0 \\ Ce^{ik_3x} + De^{-ik_3x} & 0 < x < a \quad \text{note } k_3 \end{cases}$$

$$\text{where} \begin{cases} k_1 = \dfrac{\sqrt{2mE}}{\hbar} \\ k_3 = \dfrac{\sqrt{2m(E-V_0)}}{\hbar} \end{cases}$$

Follow the method used in case 1 ($E < V_0$)

⋮

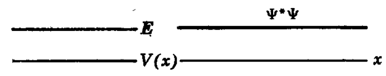
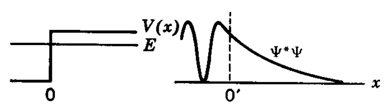
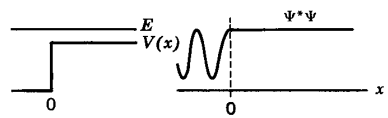
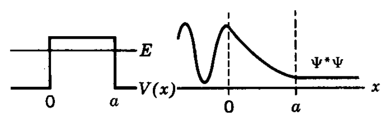
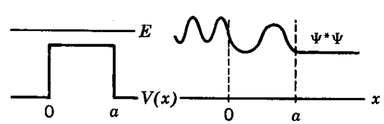
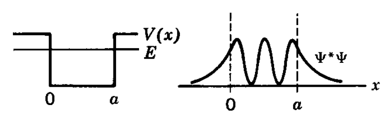
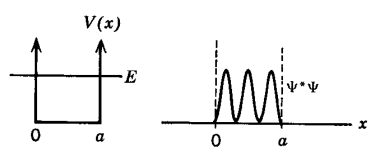
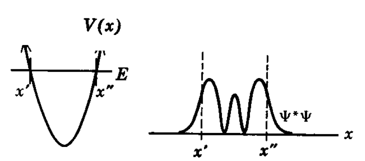
$$T = \frac{1}{1 + \dfrac{\sin^2 k_3\, a}{4\dfrac{E}{V_0}\left(\dfrac{E}{V_0} - 1\right)}}$$



Ramsauer effect:

Note if $k_3 a = \pi, 2\pi, 3\pi\ldots,$ then

$T = 1$ and $R = 0$.

Name of System	Physical Example	Potential and Total Energies	Probability Density	Significant Feature
Zero potential	Proton in beam from cyclotron			Results used for other systems
Step potential (energy below top)	Conduction electron near surface of metal			Penetration of excluded region
Step potential (energy above top)	Neutron trying to escape nucleus			Partial reflection at potential discontinuity
Barrier potential (energy below top)	α particle trying to escape Coloumb barrier			Tunneling
Barrier potential (energy above top)	Electron scattering from negatively ionized atom			No reflection at certain energies
Finite square well potential	Neutron bound in nucleus			Energy quantization
Infinite square well potential	Molecule strictly confined to box			Approximation to finite square well
Simple harmonic oscillator potential	Atom of vibrating diatomic molecule			Zero-point energy

from Eisberg and Resnick