Find the Momentum of a particle trapped in a one-dimensional box

Remember:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad n = 1, 2, 3, \ldots$$

$$\psi_n = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \qquad n = 1, 2, 3, \ldots$$

U(x) = 0, $\quad 0 < x < L$
$\quad = \infty, \quad$ elsewhere

$$\langle p\rangle = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi \, dx \quad = \int_{-\infty}^{\infty} \psi^* \left(\frac{\hbar}{i}\frac{d}{dx}\right) \psi \, dx$$

$$\psi^* = \psi_n = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}$$

$$\frac{d\psi}{dx} = \sqrt{\frac{2}{L}} \frac{n\pi}{L} \cos\frac{n\pi x}{L}$$

$$\langle p\rangle = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi \, dx \quad = \int_{-\infty}^{\infty} \psi^* \left(\frac{\hbar}{i}\frac{d}{dx}\right) \psi \, dx$$

$$= \frac{\hbar}{i} \frac{2}{L} \frac{n\pi}{L} \int_0^L \sin\frac{n\pi x}{L} \cos\frac{n\pi x}{L} \, dx$$

Note that
$$\int \sin ax \cos ax \, dx = \frac{1}{2a}\sin^2 ax$$

With $a = n\pi/L$ we have

$$\langle p\rangle = \frac{\hbar}{iL}\left[\sin^2\frac{n\pi x}{L}\right]_0^L = 0$$

since $\quad \sin^2 0 = \sin^2 n\pi = 0 \qquad n = 1, 2, 3, \ldots$

The expectation value $\langle p \rangle$ of the particle's momentum is 0.

At first glance this conclusion seems strange.

$E = p^2/2m$, and so we would anticipate that

$$p_n = \pm \sqrt{2mE_n} \quad = \pm \frac{n\pi\hbar}{L}.$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad n = 1, 2, 3, \ldots$$

The $\pm$ sign provides the explanation:

The particle is moving back and forth, so its *average* momentum for any value of n is

$$p_{av} = \frac{(+n\pi\hbar/L) + (-n\pi\hbar/L)}{2} = 0$$

the expectation value.

Remember: $$p_n = \pm \sqrt{2mE_n} \quad = \pm \frac{n\pi\hbar}{L}.$$

Looking at this expression, we anticipate that there should be TWO **momentum eigenfunctions** for every **energy eigenfunction**, corresponding to the two possible directions of motion.

The general procedure for finding the eigenvalues of a quantum-mechanical operator (here $\hat{p}$) is to start from the eigenvalue equation

$$\hat{p}\psi_n = p_n\psi_n$$

where each p_n is a real number.

This equation holds only when the wave functions ψ_n are eigenfunctions of the momentum operator $\hat{p}$,

$$\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$$

We can see at once that the energy eigenfunctions $\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$

are not also momentum eigenfunctions,

because $$\frac{\hbar}{i}\frac{d}{dx}\left(\sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}\right) = \frac{\hbar}{i}\frac{n\pi}{L}\sqrt{\frac{2}{L}} \cos \frac{n\pi x}{L}$$

$$\neq p_n\psi_n$$

To find the correct momentum eigenfunctions, we note that

$$\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i} = \frac{1}{2i}e^{i\theta} - \frac{1}{2i}e^{-i\theta}$$

Hence each energy eigenfunction can be expressed as a linear combination of the two wave functions

$$\psi_n^+ = \frac{1}{2i}\sqrt{\frac{2}{L}}\, e^{in\pi x/L}$$

$$\psi_n^- = \frac{1}{2i}\sqrt{\frac{2}{L}}\, e^{-in\pi x/L}$$

Momentum eigenfunctions for trapped particle

Inserting the first of these wave functions in the eigenvalue equation,

$$\hat{p}\psi_n^+ = p_n^+\psi_n^+$$

$$\frac{\hbar}{i}\frac{d}{dx}\psi_n^+ = \frac{\hbar}{i}\frac{1}{2i}\sqrt{\frac{2}{L}}\frac{in\pi}{L} e^{in\pi x/L} = \frac{n\pi\hbar}{L}\psi_n^+ = p_n^+\psi_n^+$$

Remember: $p_n = \pm\sqrt{2mE_n} = \pm\frac{n\pi\hbar}{L}$.

$$\boxed{p_n^+ = +\frac{n\pi\hbar}{L}}$$

Similarly the wave function ψ_n^- leads to the momentum eigenvalues

$$\boxed{p_n^- = -\frac{n\pi\hbar}{L}}$$

We conclude that ψ_n^+ and ψ_n^- are indeed the momentum eigenfunctions for a particle in a box.

The equation

$$p_n = \pm\sqrt{2mE_n} = \pm\frac{n\pi\hbar}{L}$$

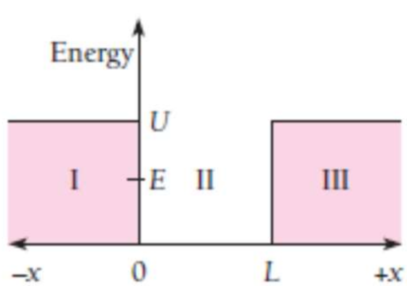
Correctly states the corresponding momentum eigenvalues.

FINITE POTENTIAL WELL

The wave function penetrates the walls, which lowers the energy levels

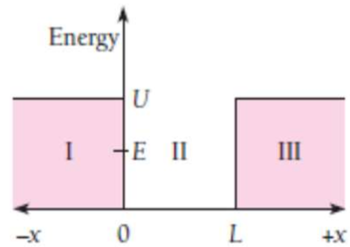
Potential energies are never infinite in the real world &
The box with infinitely hard walls has no physical counterpart.

However, potential wells with barriers of finite height certainly do exist. Let us examine the wave functions and energy levels of a particle in such a potential well.



A square potential well with finite barriers. The energy E of the trapped particle is less than the height U of the barriers.

A potential well with square corners that is *U* high and *L* wide
➔ contains a particle whose energy *E* is less than *U*.



According to classical mechanics, when the particle strikes the sides of the well, it bounces off without entering regions I and III.

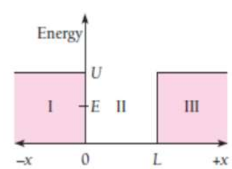
In quantum mechanics, the particle also bounces back and forth, but now it has a certain probability of penetrating into regions I and III even though ***E* < *U***.

In regions I and III Schrödinger's steady-state equation is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - U)\psi = 0$$

Time-Independent form

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - U)\psi = 0$$



which we can rewrite in the more convenient form

$$\frac{d^2\psi}{dx^2} - a^2\psi = 0 \qquad \begin{matrix} x < 0 \\ x > L \end{matrix}$$

$$\text{where} \qquad a = \frac{\sqrt{2m(U - E)}}{\hbar}$$

The solutions are

$$\psi_{\mathrm{I}} = Ce^{ax} + De^{-ax}$$

$$\psi_{\mathrm{III}} = Fe^{ax} + Ge^{-ax}$$

Both ψ_{I} and ψ_{III} must be finite everywhere.

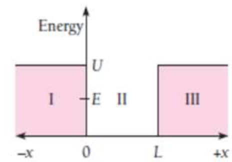
$$\left.\begin{matrix} \text{Since } e^{-ax} \to \infty \text{ as } x \to -\infty \\ \text{and } e^{ax} \to \infty \text{ as } x \to \infty \end{matrix}\right\}$$

the coefficients D and F must therefore be 0.

Hence we have

$$\psi_{\mathrm{I}} = Ce^{\alpha x}$$
$$\psi_{\mathrm{III}} = Ge^{-\alpha x}$$

These wave functions decrease exponentially inside the barriers at the sides of the well.



$$\psi_{\mathrm{I}} = Ce^{\alpha x} + De^{-\alpha x}$$
$$\psi_{\mathrm{III}} = Fe^{\alpha x} + Ge^{-\alpha x}$$

Within the well, Schrödinger's equation is the same as earlier (infinite well), and its solution is again

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

$$\psi_{\mathrm{II}} = A \sin\frac{\sqrt{2mE}}{\hbar}x + B \cos\frac{\sqrt{2mE}}{\hbar}x$$

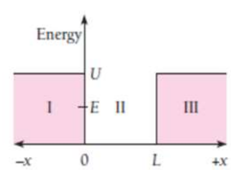
In the case of a well with infinitely high barriers, we found that $B = 0$ in order that $\psi = 0$ at $x = 0$ and $x = L$

Here, however, $\psi_{\mathrm{II}} = C$ at $x = 0$ and $\psi_{\mathrm{II}} = G$ at $x = L$, so both the sine and cosine solutions are possible.

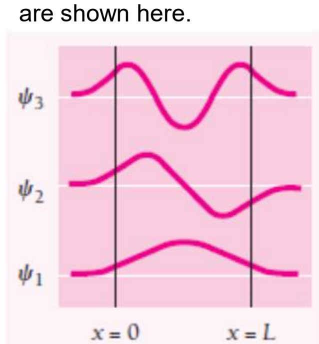
For either solution, both ψ and $d\psi/dx$ must be continuous at $x = 0$ and $x = L$:

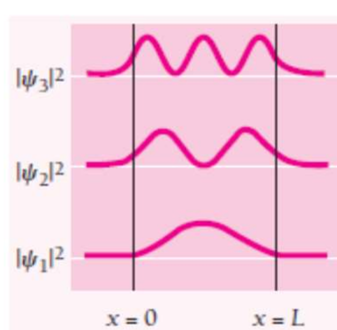
The wave functions inside and outside each side of the well must not only have the same value where they join, but also the same slopes, so they match up perfectly.

When these boundary conditions are taken into account, the result is that exact matching only occurs for certain specific values E_n of the particle energy.



The complete wave functions and their probability densities are shown here.

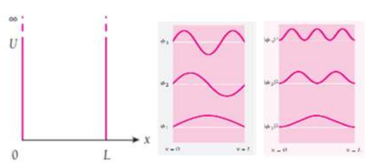




Because the wavelengths that fit into the well are longer than for an infinite well of the same width, the corresponding particle momenta are lower (recall that $\lambda = h / p$).

Hence, the energy levels E_n are lower for each n than they are for a particle in an infinite well.

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad n = 1, 2, 3, \ldots}$$



INFINITE POTENTIAL WELL

U(x) = 0, $0 < x < L$

= ∞, elsewhere

wave function ψ is 0 for $x \leq 0$ and $x \geq L$.

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

$$\psi = A \sin\frac{\sqrt{2mE}}{\hbar}x + B\cos\frac{\sqrt{2mE}}{\hbar}x$$

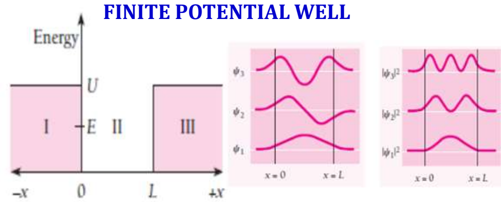
$\psi = 0$ for $x = 0$ $\Longrightarrow$ B = 0

$$\psi = A \sin\frac{\sqrt{2mE}}{\hbar}x$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad n = 1, 2, 3, \ldots$$

$$\psi_n = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \qquad n = 1, 2, 3, \ldots$$

FINITE POTENTIAL WELL



In regions I and III $\quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - U)\psi = 0$

$$\frac{d^2\psi}{dx^2} - a^2\psi = 0 \qquad \begin{matrix} x < 0 \\ x > L \end{matrix} \qquad a = \frac{\sqrt{2m(U - E)}}{\hbar}$$

$$\psi_I = Ce^{ax} \qquad \psi_{III} = Ge^{-ax}$$

These wave functions decrease exponentially inside the barriers at the sides of the well.

Within the well, it is the same as earlier (infinite well), and its solution is again

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \qquad \psi_{II} = A \sin\frac{\sqrt{2mE}}{\hbar}x + B\cos\frac{\sqrt{2mE}}{\hbar}x$$

Here, however, $\psi_{II} = C$ at $x = 0$ and $\psi_{II} = G$ at $x = L$, , so both the sine and cosine solutions are possible.

The wavelengths are longer than for an infinite well of the same width, corresponding particle momenta are lower ($\lambda = h/p$).

E_n are lower for each n compared to the infinite well

Example 5.5

Find the expectation value $\langle x \rangle$ of the position of a particle trapped in a box L wide.

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\psi|^2\, dx \quad = \frac{2}{L}\int_0^L x \sin^2 \frac{n\pi x}{L}\, dx$$

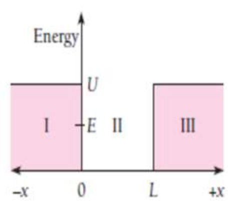
$$= \frac{2}{L}\left[\frac{x^2}{4} - \frac{x \sin(2n\pi x/L)}{4n\pi/L} - \frac{\cos(2n\pi x/L)}{8(n\pi/L)^2}\right]_0^L$$

Since $\sin n\pi = 0$, $\cos 2n\pi = 1$, and $\cos 0 = 1$, for all the values of n the expectation value of x is

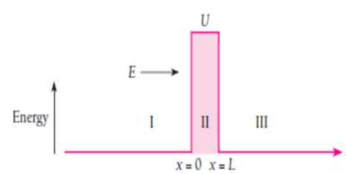
$$\langle x \rangle = \frac{2}{L}\left(\frac{L^2}{4}\right) = \frac{L}{2}$$

This result means that the average position of the particle is the middle of the box in all quantum states. There is no conflict with the fact that $|\psi|^2 = 0$ at $L/2$ in the $n = 2, 4, 6, \ldots$ states because $\langle x \rangle$ is an *average*, not a probability, and it reflects the symmetry of $|\psi|^2$ about the middle of the box.

- ✓ **Although the walls of the potential well were of finite height (FINITE POTENTIAL WELL), they were assumed to be infinitely thick.**
- ✓ **As a result, the particle was trapped forever, even though it could penetrate the walls.**



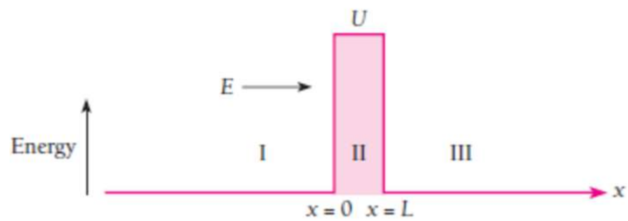
- ✓ **We next examine the situation of a particle that strikes a potential barrier of height U, again with E < U, but this time the barrier has a finite width.**
- ✓ **What we will find is that the particle has a certain probability—not necessarily great, but not zero either—of passing through the barrier and emerging on the other side.**
- ✓ **The particle lacks the energy to overcome the top of the barrier, but it can still tunnel through it.**



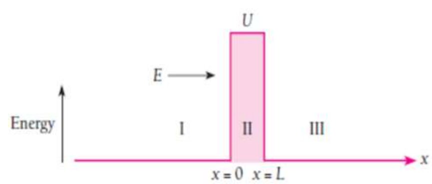
No surprise, the higher the barrier and the wider it is, the less the chance that the particle can get through.

The **tunnel effect** actually occurs, notably in the case of alpha particles emitted by certain radioactive nuclei.

One-Dimensional barrier potential



$$V(x) = \begin{cases} 0 & x < 0 \\ U & 0 < x < L \\ 0 & x > L \end{cases}$$

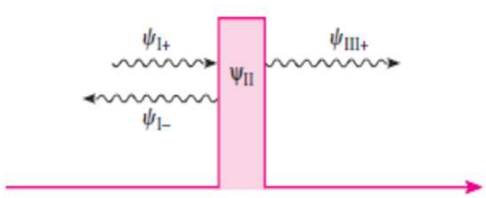


$$V(x) = \begin{cases} 0 & x < 0 \\ U & 0 < x < L \\ 0 & x > L \end{cases}$$

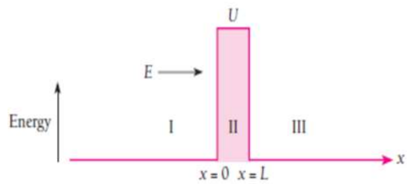
Energy of the particle E < barrier height U

Classical Mechanics: No probability of finding the particle in regions II and III
The particle is reflected

Quantum Mechanical: Set up the Schrödinger equation in three regions
Find the wavefunctions



ψ_{I+} represents the incoming particles
ψ_{I-} represents the reflected particles
ψ_{III} represents the transmitted particles
ψ_{II} represents the particles inside the barrier, some of which end up in region III while the others return to region I.



Schrödinger equations in regions I and III

$$\frac{d^2\psi_{I}}{dx^2} + \frac{2m}{\hbar^2}E\psi_{I} = 0$$

$$\frac{d^2\psi_{III}}{dx^2} + \frac{2m}{\hbar^2}E\psi_{III} = 0$$

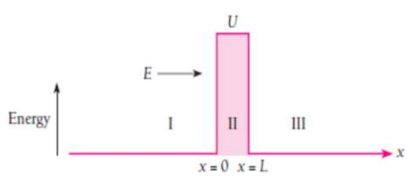
Solutions :

$$\psi_{I} = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_{III} = Fe^{ik_1x} + Ge^{-ik_1x}$$

where

Wave number outside barrier $\quad k_1 = \frac{\sqrt{2mE}}{\hbar} = \frac{p}{\hbar} = \frac{2\pi}{\lambda}$



Incoming wave $\quad \psi_{I+} = Ae^{ik_1x}$

Reflected wave $\quad \psi_{I-} = Be^{-ik_1x}$

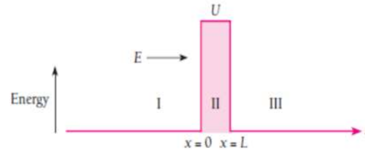
$$\psi_{I} = \psi_{I+} + \psi_{I-}$$

On the far side of the barrier ($x > L$) there can only be a

Transmitted wave $\quad \psi_{III+} = Fe^{ik_1x}$

since region III contains nothing that could reflect the wave. Hence $G = 0$

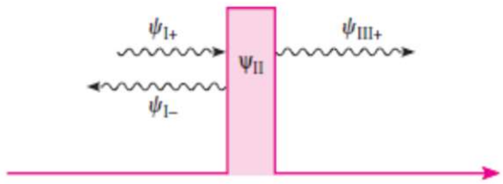
$$\psi_{III} = \psi_{III+} = Fe^{ik_1x}$$



Incoming wave $\psi_{I+} = Ae^{ik_1 x}$

Reflected wave $\psi_{I-} = Be^{-ik_1 x}$

Transmitted wave $\psi_{III+} = Fe^{ik_1 x}$



The **transmission probability *T*** for a particle to pass through the barrier is equal to the fraction of the incident beam that gets through the barrier.

Incoming wave $\psi_{I+} = Ae^{ik_1 x}$

This wave corresponds to the incident beam of particles in the sense that $|\psi_{I+}|^2$ is their probability density. If v_{I+} is the group velocity of the incoming wave, which equals the velocity of the particles, then

$$S = |\psi_{I+}|^2 v_{I+}$$

v_{I+} is the group velocity of the incoming wave

is the flux of particles that arrive at the barrier. That is, S is the number of particles per second that arrive there.

The transmission probability T for a particle to pass through the barrier is the ratio

$$T = \frac{|\psi_{III+}|^2 v_{III+}}{|\psi_{I+}|^2 v_{I+}} = \frac{FF^* v_{III+}}{AA^* v_{I+}}$$

HOW?

between the flux of particles that emerges from the barrier and the flux that arrives at it. In other words, T is the fraction of incident particles that succeed in tunneling through the barrier. Classically $T = 0$ because a particle with $E < U$ cannot exist inside the barrier; let us see what the quantum-mechanical result is.

Transmission Coefficient T

$$= \frac{Transmited\ probability\ current\ density\ (J_t)}{incidentprobability\ current\ density(J_{in})}$$

$$J_{in} = \frac{\hbar}{2mi}[\Psi_{in}^* \frac{d\Psi_{in}}{dx} - \frac{d\Psi_{in}^*}{dx}\Psi_{in}]$$

$$\Psi_{in} = Ae^{-i(\omega t - k_1 x)} \qquad \Psi_{in}^* = Ae^{i(\omega t - k_1 x)}$$

$$J_{in} = \frac{\hbar}{2mi}[ik_1|A|^2 - (-ik_1|A|^2)]$$

$$= \frac{\hbar k_1}{m}\ |A|^2$$

$$= v_I|A|^2$$

Transmission Coefficient T

$$= \frac{Transmited\ probability\ current\ density\ (J_t)}{incidentprobability\ current\ density(J_{in})}$$

$$J_{in} = \frac{\hbar}{2mi}\left[\Psi_{in}^* \frac{d\Psi_{in}}{dx} - \frac{d\Psi_{in}^*}{dx}\Psi_{in}\right] = v_I|A|^2$$

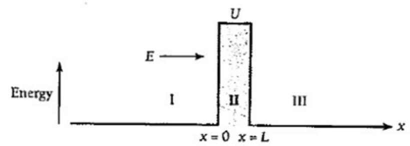
Similarly

$$\Psi_{tr} = Fe^{-i(\omega t - k_1 x)} \quad (v_{III} = v_I)$$

$$J_{tr} = \frac{\hbar k_1}{m}|F|^2$$

$$= v_{III}|F|^2$$

Transmission Coefficient: $T = \frac{|F|^2 v_{III}}{|A|^2 v_I} = \left|\frac{F}{A}\right|^2$



In region II Schrödinger's equation for the particles is

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2}(E-U)\psi_{II} = \frac{d^2\psi_{II}}{dx^2} - \frac{2m}{\hbar^2}(U-E)\psi_{II} = 0$$

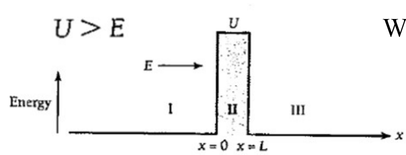
Since $U > E$ the solution is

Wave function inside barrier $\psi_{II} = Ce^{-k_2 x} + De^{k_2 x}$

where the wave number inside the barrier is

Wave number inside barrier $k_2 = \frac{\sqrt{2m(U-E)}}{\hbar}$

$U > E$



Wavefunctions :

$$\psi_I = Ae^{ik_1 x} + Be^{-ik_1 x}$$
$$\psi_{II} = Ce^{-k_2 x} + De^{k_2 x}$$
$$\psi_{III} = \psi_{III+} = Fe^{ik_1 x}$$

Applying the Boundary Conditions

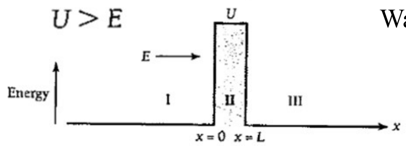
Boundary conditions at $x = 0$

$$\left.\begin{aligned} \psi_I &= \psi_{II} \\ \frac{d\psi_I}{dx} &= \frac{d\psi_{II}}{dx} \end{aligned}\right\} x = 0$$

Boundary conditions at $x = L$

$$\left.\begin{aligned} \psi_{II} &= \psi_{III} \\ \frac{d\psi_{II}}{dx} &= \frac{d\psi_{III}}{dx} \end{aligned}\right\} x = L$$

$U > E$



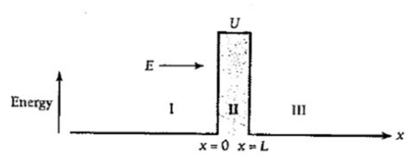
Wavefunctions :

$$\psi_I = Ae^{ik_1x} + Be^{-ik_1x}$$
$$\psi_{II} = Ce^{-k_2x} + De^{k_2x}$$
$$\psi_{III} = \psi_{III+} = Fe^{ik_1x}$$

Applying the Boundary Conditions

$$\left.\begin{aligned} \psi_I &= \psi_{II} \\ \frac{d\psi_I}{dx} &= \frac{d\psi_{II}}{dx} \end{aligned}\right\} x = 0 \qquad \begin{aligned} A + B &= C + D \\ ik_1A - ik_1B &= -k_2C + k_2D \end{aligned}$$

$$\left.\begin{aligned} \psi_{II} &= \psi_{III} \\ \frac{d\psi_{II}}{dx} &= \frac{d\psi_{III}}{dx} \end{aligned}\right\} x = L \qquad \begin{aligned} Ce^{-k_2L} + De^{k_2L} &= Fe^{ik_1L} \\ -k_2Ce^{-k_2L} + k_2De^{k_2L} &= ik_1Fe^{ik_1L} \end{aligned}$$



In region II Schrödinger's equation for the particles is

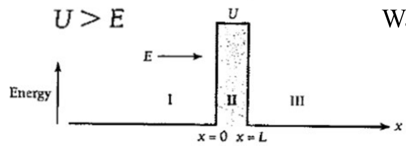
$$\frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2}(E - U)\psi_{II} = \frac{d^2\psi_{II}}{dx^2} - \frac{2m}{\hbar^2}(U - E)\psi_{II} = 0$$

Since $U > E$ the solution is $\psi_{II} = Ce^{-k_2x} + De^{k_2x}$

where the wave number inside the barrier is $k_2 = \dfrac{\sqrt{2m(U - E)}}{\hbar}$

Since the exponents are real quantities, ψ_{II} does not oscillate and therefore does not represent a moving particle. However, the probability density $|\psi_{II}|^2$ is not zero, so there is a finite probability of finding a particle within the barrier. Such a particle may emerge into region III or it may return to region I.

$U > E$



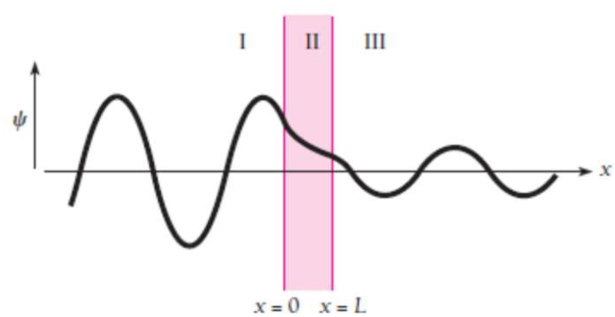
Wavefunctions :

$$\psi_{\mathrm{I}} = Ae^{ik_1x} + Be^{-ik_1x}$$
$$\psi_{\mathrm{II}} = Ce^{-k_2x} + De^{k_2x}$$
$$\psi_{\mathrm{III}} = \psi_{\mathrm{III}+} = Fe^{ik_1x}$$

Applying the Boundary Conditions

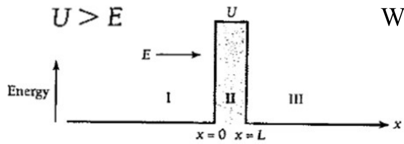
$$A + B = C + D$$
$$ik_1A - ik_1B = -k_2C + k_2D$$
$$Ce^{-k_2L} + De^{k_2L} = Fe^{ik_1L}$$
$$-k_2Ce^{-k_2L} + k_2De^{k_2L} = ik_1Fe^{ik_1L}$$

$$\boxed{\left(\frac{A}{F}\right) = \left[\frac{1}{2} + \frac{i}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\right]e^{(ik_1+k_2)L} + \left[\frac{1}{2} - \frac{i}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\right]e^{(ik_1-k_2)L}}$$



At each wall of the barrier, the wave functions inside and outside it must match perfectly, meaning they must have the same values and slopes.

$U > E$



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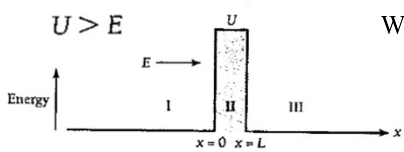
$$k_1 = \frac{\sqrt{2mE}}{\hbar} \qquad k_2 = \frac{\sqrt{2m(U-E)}}{\hbar}$$

Approximation 1 : ***U* >> *E*** $\quad k_2/k_1 > k_1/k_2 \qquad \frac{k_2}{k_1} - \frac{k_1}{k_2} \approx \frac{k_2}{k_1}$

Approximation 2 : ***barrier is wide (large L)*** $\quad k_2L \gg 1 \qquad e^{k_2L} \gg e^{-k_2L}$

$$\left(\frac{A}{F}\right) = \left(\frac{1}{2} + \frac{ik_2}{4k_1}\right)e^{(ik_1+k_2)L} \qquad \left(\frac{A}{F}\right)^* = \left(\frac{1}{2} - \frac{ik_2}{4k_1}\right)e^{(-ik_1+k_2)L}$$

$U > E$



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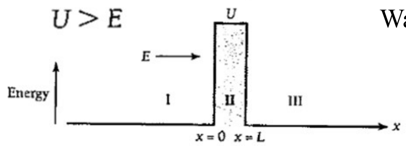
$$\frac{AA^*}{FF^*} = \left(\frac{1}{4} + \frac{k_2^2}{16k_1^2}\right)e^{2k_2L} \qquad v_{III+} = v_{I+}$$

Transmission probability $\quad T = \frac{FF^*v_{III+}}{AA^*v_{I+}} = \left(\frac{AA^*}{FF^*}\right)^{-1} = \left[\frac{16}{4 + (k_2/k_1)^2}\right]e^{-2k_2L}$



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$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad k_2 = \frac{\sqrt{2m(U-E)}}{\hbar}$$

$$\left(\frac{k_2}{k_1}\right)^2 = \frac{2m(U-E)/\hbar^2}{2mE/\hbar^2} = \frac{U}{E} - 1$$

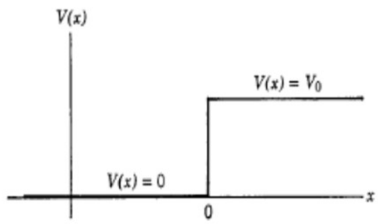
Transmission probability $T = \dfrac{FF^* v_{III+}}{AA^* v_{I+}} = \left(\dfrac{AA^*}{FF^*}\right)^{-1} = \left[\dfrac{16}{4 + (k_2/k_1)^2}\right] e^{-2k_2L}$

- ✓ This formula means that the quantity in brackets **varies much less with *E* and *U* than does the exponential**.
- ✓ The bracketed quantity, furthermore, is always of the order of magnitude of 1 in value.

A reasonable approximation of the transmission probability is therefore

Approximate transmission probability $T = e^{-2k_2L}$

THE STEP POTENTIAL (ENERGY LESS THAN STEP HEIGHT)

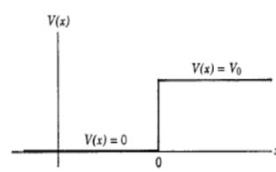


A step potential.

$$V(x) = \begin{cases} V_0 & x > 0 \\ 0 & x < 0 \end{cases}$$

- ✓ Assume that a particle of mass ***m*** and total energy ***E*** is in the region $x < 0$, and that it is moving toward the point $x = 0$ at which the step potential $V(x)$ abruptly changes its value.
- ✓ According to classical mechanics, particle will move freely in that region until it reaches $x = 0$, where it is subjected to an impulsive force $F = - dV(x)/dx$ acting in the direction of decreasing x.

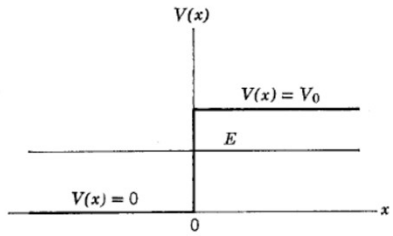
- ✓ The idealized potential yields an impulsive force of infinite magnitude acting only at the point $x = 0$.
- ✓ However, as it acts on the particle only for an infinitesimal time, the quantity $\int F\,dt$ (the impulse), which determines the change in its momentum, is finite.
- ✓ In fact, the momentum change is not affected by the idealization.



$$V(x) = \begin{cases} V_0 & x > 0 \\ 0 & x < 0 \end{cases}$$

- ✓ **The motion of the particle subsequent to experiencing the force at x = 0 depends, in classical mechanics, on the relation between E and V_0 .**
- ✓ **This is also true in quantum mechanics.**

We treat the case where E < Vo , where the total energy is less than the height of the potential step



For the step potential, the x axis breaks up into two regions. In the region where $x < 0$ (left of the step), we have $V(x) = 0$, so the eigenfunction that will tell us about the behavior of the particle is a solution to the simple time-independent Schroedinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad x < 0$$

In the region where $x > 0$ (right of the step), we have $V(x) = V_0$, and the eigenfunction is a solution to a time-independent Schroedinger equation which is almost as simple

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x) \qquad x > 0$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad x < 0$$

Since this is precisely the time-independent Schroedinger equation for a free particle, we take for its *general* solution the traveling wave eigenfunction

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad \text{where } k_1 = \frac{\sqrt{2mE}}{\hbar} \qquad x < 0$$

- ✓ Next, consider the differential equation valid for the region in which $V(x) = V_0$
- ✓ From the qualitative considerations, we do not expect an oscillatory function to be a solution since the total energy E < Vo in the region of interest.
- ✓ The simplest function with this property is the decreasing *real* exponential,

$$\psi(x) = Ce^{k_2x} + De^{-k_2x} \qquad \text{where } k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \qquad x > 0$$

TRY this at home

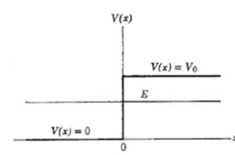
Find out if following is a solution and, if so, also find the required value of k_2

$$\psi(x) = e^{-k_2 x} \qquad x > 0$$

This satisfies the equation, and therefore verifies the solution, providing

$$k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \qquad E < V_0$$

The arbitrary constants *A, B, C,* and *D* must be so chosen that the total eigenfunction satisfies the requirements concerning finiteness, single-valuedness, and continuity of $\psi(x)$ and $d\psi(x)/dx$.



Consider first the behavior of $\psi(x)$ as $x \to +\infty$. Inspection shows that it will generally increase without limit as $x \to +\infty$, because of the presence of the first term, Ce^{k2x}.

In order to prevent this, and keep $\psi(x)$ finite, we must set the arbitrary coefficient C = 0

Continuity of $\psi(x)$ is obtained by satisfying the relation

$$D(e^{-k_2 x})_{x=0} = A(e^{ik_1 x})_{x=0} + B(e^{-ik_1 x})_{x=0}$$

which comes from equating the two forms at $x = 0$. This relation yields

$$D = A + B$$

Continuity of the derivative of the two forms

$$\frac{d\psi(x)}{dx} = -k_2 D e^{-k_2 x} \qquad x > 0$$

and

$$\frac{d\psi(x)}{dx} = ik_1 A e^{ik_1 x} - ik_1 B e^{-ik_1 x} \qquad x < 0$$

is obtained by equating these derivatives at $x = 0$. Thus we set

$$-k_2 D(e^{-k_2 x})_{x=0} = ik_1 A(e^{ik_1 x})_{x=0} - ik_1 B(e^{-ik_1 x})_{x=0}$$

This yields

$$\frac{ik_2}{k_1} D = A - B$$

Adding & Subtracting gives $D = A + B$ & $\frac{ik_2}{k_1} D = A - B$

$$A = \frac{D}{2}\left(1 + \frac{ik_2}{k_1}\right) \qquad B = \frac{D}{2}\left(1 - \frac{ik_2}{k_1}\right)$$

We have now determined A, B, and C in terms of D. Thus the eigenfunction for the step potential, and for the energy $E < V_0$, is

$$\psi(x) = \begin{cases} \frac{D}{2}(1 + ik_2/k_1)e^{ik_1 x} + \frac{D}{2}(1 - ik_2/k_1)e^{-ik_1 x} & x \leq 0 \\ De^{-k_2 x} & x \geq 0 \end{cases}$$

To calculate the probability that the incident particle is reflected, which we call the *reflection coefficient R.*

Obviously, *R* depends on the ratio *B/A,* which specifies the amplitude of the reflected part of the wave function relative to the amplitude of the incident part.

But in quantum mechanics, probabilities depend on intensities, such as *B*B* and *A*A,* not on amplitudes.

Thus, we must evaluate *R* from the formula

$$R = \frac{B^*B}{A^*A}$$

$$R = \frac{B^*B}{A^*A}$$

$$R = \frac{B^*B}{A^*A} = \frac{(1 - ik_2/k_1)^*(1 - ik_2/k_1)}{(1 + ik_2/k_1)^*(1 + ik_2/k_1)}$$

$$R = \frac{(1 + ik_2/k_1)(1 - ik_2/k_1)}{(1 - ik_2/k_1)(1 + ik_2/k_1)} = 1 \qquad\qquad E < V_0$$

The fact that this ratio equals one means that a particle incident upon the potential step, with total energy less than the height of the step, has probability one of being reflected—it is always reflected. This is in agreement with the predictions of classical mechanics.

Consider now the eigenfunction

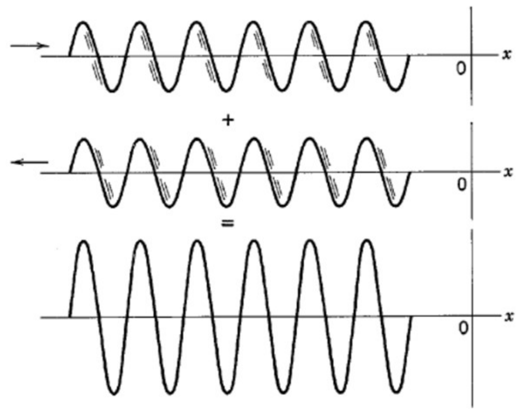
$$\psi(x) = \begin{cases} \frac{D}{2}(1 + ik_2/k_1)e^{ik_1x} + \frac{D}{2}(1 - ik_2/k_1)e^{-ik_1x} & x \le 0 \\ De^{-k_2x} & x \ge 0 \end{cases}$$

Using the relation $e^{ik_1x} = \cos k_1x + i \sin k_1x$

the eigenfunction can be expressed as

$$\psi(x) = \begin{cases} D\cos k_1x - D\dfrac{k_2}{k_1}\sin k_1x & x \le 0 \\ De^{-k_2x} & x \ge 0 \end{cases}$$

If we generate the wave function by multiplying $\psi(x)$ by $e^{-iEt/\hbar}$, we see immediately that we actually have a standing wave because the locations of the nodes do not change in time. In this problem the incident and reflected traveling waves for $x < 0$ combine to form a standing wave because they are of equal intensity.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