Single Step Barrier

(Other names: Potential Step, Barrier Penetration)

Consider

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

Case $E < V_0$

Classically

$$E = \frac{p^2}{2m} + V_0$$

$$p^2 = 2m(E - V_0)$$

Since $E < V_0$ thus $p^2 < 0$ which is not possible. Thus the particle cannot e found in region $x > 0$ according to classical mechanics. The particle would be reflected back at x=0 because it does not have sufficient energy to climb the barrier. On the other hand if $> V_0$, then the particle would not be reflected; it would keep moving towards the right with reduced energy.

Quantum mechanical consideration

Since V is independent of time

$$\psi(x,t) = \psi(x)\psi(t)$$

$$\psi(x,t) = \psi(x)e^{-i\frac{Et}{\hbar}}$$

Substituting in

$$\mathrm{i}\hbar\frac{\partial\psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t)$$

$$\mathrm{i}\hbar\left(\frac{-\mathrm{iE}}{\hbar}\right)\psi(x) = \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x)$$

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

Known as time independent Schrödinger equation

Substituting $V(x)$ from above

$$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2mE}{\hbar^2}\psi(x)=0 \qquad for\ x<0$$

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

Let

$$k_1^2=\frac{2mE}{\hbar^2}\,k_2^2=\frac{2m}{\hbar^2}(E-V_0)$$

$$\frac{\partial^2\psi(x)}{\partial x^2}+k_1^2\psi(x)=0 \qquad for\ x<0$$

$$\frac{\partial^2\psi(x)}{\partial x^2}+k_2^2\psi(x)=0 \qquad for\ x>0$$

$$\psi(x)=Ae^{ik_1x}+Be^{-ik_1x} \qquad for\ x<0$$

$$\psi(x)=Ce^{ik_2x}+De^{-ik_2x} \qquad for\ x>0$$

The term Ae^{ik_1x} represents the wave travelling in the positive x-direction in the first region and the second term represents the reflected part of the incident wave travelling in the negative x-direction in the first region.

Similarly, the term Ce^{ik_1x} represents the wave travelling in the positive x-direction in the second region and the second term represents the reflected part of the transmitted wave travelling in the negative x-direction in the second region. Since, discontinuity occurs only at x=0 in the region II and after which there occurs no discontinuity in this region. This mean that the reflection will not take place in this region, i.e. D=0.

$$\psi(x)=\begin{cases}Ae^{ik_1x}+Be^{-ik_1x} & for\ x<0\\ Ce^{ik_2x} & for\ x>0\end{cases}$$

Solving for A , B ,and C

$$\lim_{x\to 0^-}\psi(x)=\lim_{x\to 0^+}\psi(x)$$

$$\psi(0^-)=A+B=\psi(0^+)=C$$

$$A + B = C$$

Again

$\left.\frac{d\psi(x)}{dx}\right|_{x=0}$ must be continuous

$$\left.\frac{d\psi(x)}{dx}\right|_{x=0^-} = Aik_1 - Bik_1$$

$$\left.\frac{d\psi(x)}{dx}\right|_{x=0^+} = Cik_2$$

$$Aik_1 - Bik_1 = Cik_2$$

Solving

$$A + B = C$$

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

$$B = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)A$$

$$C = \left(\frac{2k_1}{k_1 + k_2}\right)A$$

Substituting back in

$$\psi(x) = A\left(e^{ik_1x} + \left(\frac{k_1 - k_2}{k_1 + k_2}\right)e^{-ik_1x}\right) \qquad for\ x < 0$$

Incident wave + reflected wave

$$\psi(x) = A\left(\frac{2k_1}{k_1 + k_2}\right)e^{-ik_2x} \qquad for\ x > 0$$

Transmitted wave

Probability of finding the particle in region $x > 0$

The probability current density

Reflectance, Reflectivity or reflection coefficient

Version 3.5

For certain applications, for example the potential step problem, it is useful to introduce a quantity called the probability current density. It is defined as

$$J(x,t) = \frac{\hbar}{2im}\left(\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right) = Re\left[\psi^*\frac{\hbar}{im}\frac{\partial\psi}{\partial x}\right]$$

The above quantity can be thought of as product of velocity and probability density.

$$\text{Reflectance } |R| = \frac{J_{reflected}}{J_{incident}}$$

$$\text{Transmittance } |T| = \frac{J_{transmitted}}{J_{incident}}$$

$$J_{incident} = \frac{\hbar k_1}{m}|A|^2, J_{reflected} = \frac{\hbar k_1}{m}|B|^2, J_{transmitted} = \frac{\hbar k_2}{m}|C|^2$$

$$R = \left|\frac{B}{A}\right|^2 = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2$$

$$T = \left|\frac{C}{A}\right|^2 = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

Substituting the values of k_1 and k_2, for$E > V_0$ and simplifying the above become

$$R = \left(\frac{1 - \left(1 - \frac{V_0}{E}\right)^{\frac{1}{2}}}{1 + \left(1 - \frac{V_0}{E}\right)^{\frac{1}{2}}}\right)^2$$

$$T = \frac{4\left(1 - \frac{V_0}{E}\right)^{\frac{1}{2}}}{\left(1 + \left(1 - \frac{V_0}{E}\right)^{\frac{1}{2}}\right)^2}$$

Note that R and T depend only on the ratio $\frac{V_0}{E}$. Note also that $R + T = 1$ as it must be, because the probability is conserved.

Case $E < V_0$

Version 3.5

Let us define a positive real number α such that $\alpha = ik_2$

Thus the second differential equation will become:

$$\frac{\partial^2\psi(x)}{\partial x^2} - \alpha^2\psi(x) = 0 \qquad for\ x > 0$$

and the solution will be

$$\psi(x) = Ce^{-\alpha x} + De^{\alpha x} \qquad for\ x > 0$$

The wave function should not become ∞ as $x \to \infty$, thus we must choose D=0.

$$\psi(x) = Ce^{-\alpha x} \qquad for\ x > 0$$

Note that he wave function is non zero in the classically forbidden region II, although it decreases rapidly as *x* increases.

Thus, there is a finite, though small, probability of finding a particle in region II. This phenomenon is called barrier penetration or tunnel effect.

Here

$$R = \left|\frac{k_1 - i\alpha}{k_1 + i\alpha}\right|^2 = 1$$

Since the eigenfunction is now real in region II, the transmitted probability current is zero.

$$T = 0$$

Thus the probability of finding the particle in the region $x > 0$ will be

$$\psi(x)\psi^*(x) = A^2\frac{k_1^2}{k_1^2+\alpha^2}e^{-2\alpha x}$$

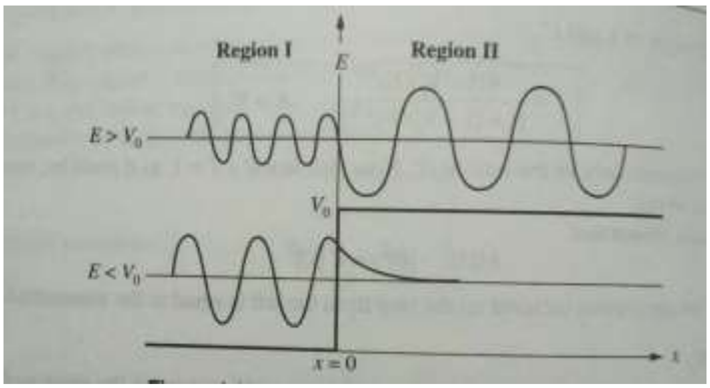
The finite probability of finding the particle in classically forbidden region is known as **tunnel effect.**

In the limit of large energies $E \gg V_0$, we have $k_1 \approx k_2$and the classical result $R = 1$,$T = 0$is recovered.

Although, there is a finite probability of finding the particle in the classically-forbidden region, there is no permanent penetration. It means that there is a continuous reflection in the second region until all incident particle are returned to first region.

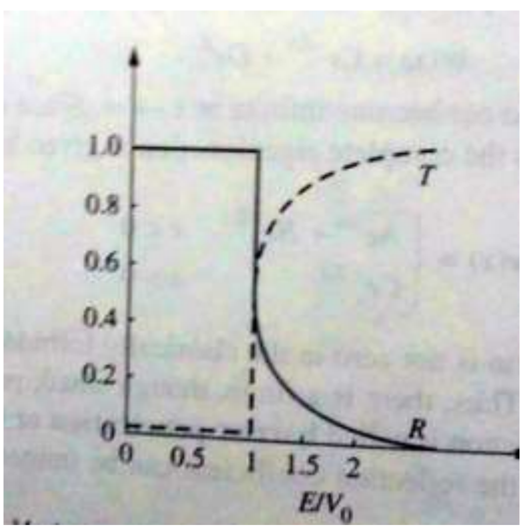
The transmission of particles even when the particle energy is less than the barrier height is known as barrier penetration or tunnel effect. It is a unique quantum phenomenon and illustrates a fundamental difference between classical and quantum physics. Tunnel effect in barriers of finite width is used to explain various phenomena in atomic, nuclear and solid state physics.

For E > V_0, the wavefunctions are given below. The reason for the larger amplitude in the second region is that the particle spends more time there because of the slow speed. The wavelength is also larger because the kinetic energy is lower.



For E < Vo, the wave function is exponentially deceasing but nonzero is region II.

The variation of reflection and transmission coefficients as a function of E/Vo is given below.



A physical example of the above problem can be thought as the neutron which is trying to escape nucleus. Here we assume that the energy of the incident particle is greater than the step barrier height. The wavelength of the particle suddenly changes from first region to second region.

$$\lambda_1 = \frac{h}{\sqrt{2mE}} \text{ to } \lambda_2 = \frac{h}{\sqrt{2m(E-V_0)}}$$

Hence, a small part of the wave associated with the particle is reflected due to this change in wavelength and the rest part is transmitted.

Momentum Operator, Energy Operator, Expectation Value

$$\hat{p} = -\hbar\frac{\partial}{\partial x}$$

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

$$\int_{-\infty}^{\infty} x\,|\psi(x)|^2 dx$$

Hamiltonian

An operator to be applied to total energy of the system

$$\widehat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$$

Thus for a free particle not bounded by any potential

$$\widehat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

For constant potential well

$$\widehat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0$$

For a simple harmonic oscillator

$$\widehat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2 x^2}{2}$$

For a hydrogen atom electron

$$\widehat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{1}{4\pi\varepsilon_0}\frac{me^2}{r^2}$$

The above operator can be applied to $\psi(x)$, the wave function. The Equation will look like

$$\hat{H}\psi(x) = E\psi(x)$$

Which is same as an eigenvalue equation. The Energy values of the above equations are eigenvalues.

Tutorial Questions

1. The wave function of a particle is $\psi(x) = A\cos^2 x$ for the interval $-\frac{\pi}{2}$ to $\frac{\pi}{2}$. Find the value of A.
2. A particle limited to the x-axis has a the wave function $\psi(x) = ax$ between x=0 and x=1. $\psi(x) = 0$ elsewhere. Find the (a) the probability that the particle can be found between x=0.45 and the expectation value $< x >$of the particle's position.
3. Explain analytically how quantum mechanical tunneling depends on the width of the potential barrier.
4. Calculate the transmittance and reflectance for a quantum mechanical particle striking a potential barrier V_0. Hence find T+R.
5. Discuss the significance of Zero point energy in Quantum mechanics.