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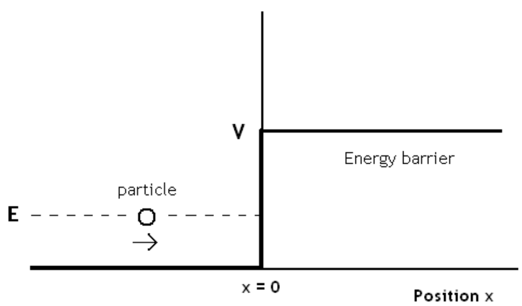
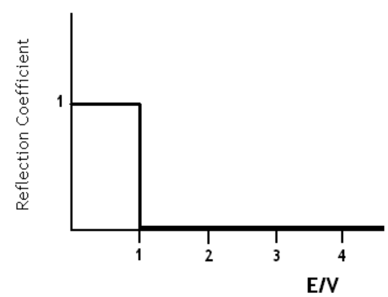
Problem Statement

As suggested by Scott Campbell

The model shown below describes a situation in which a particle of energy (E) is "shot" at an energy barrier (infinite in the positive x direction) with potential (V). If the reflection coefficient is defined to be the probability that the particle will be reflected by the barrier, the classical reflection coefficient would look like that shown in the right hand figure – any particle with energy less than V will be reflected and any with energy greater than V will pass into the barrier. For very small particles, quantum mechanics, rather than classical mechanics, is the accurate description of the particle's behavior – and it yields a different result.





For the situation shown above, the quantum mechanical description of the particle's behavior is given by the following forms of the Schrödinger equation:

$$\frac{h^2}{8\pi^2 m}\frac{d^2\Psi_1}{dx^2} = -E\Psi_1 \qquad x < 0 \qquad (1)$$

$$\frac{h^2}{8\pi^2 m}\frac{d^2\Psi_2}{dx^2} = -(E-V)\Psi_2 \qquad x \geq 0 \qquad (2)$$

where Ψ_1 and Ψ_2 are the wave functions for the particle for $x < 0$ and $x \geq 0$, respectively, E is the particle energy, m is the particle mass, V is the potential height of the barrier and h is Planck's constant.

The goal of this project was to evaluate the reflection coefficient for the quantum mechanical description (for the case of $E > V$).

The first objective was to prove that, for suitable choices of *r* and *k*,

$$\Psi_1 = A_1 e^{irx} + B_1 e^{-irx} \qquad \Psi_2 = A_2 e^{ikx} + B_2 e^{-ikx}$$

were solutions to the Schrödinger equations (1) and (2) where A_1, B_1, A_2 and B_2 are unknown constants. Also, explicit expressions for *r* and *k* were found.

The second objective was to evaluate the reflection coefficient, defined as

$$\frac{|B_1|^2}{|A_1|^2}.$$

In the above wave equations for Ψ_1 and Ψ_2, the terms e^{irx} and e^{ikx} represent a particle moving to the right (with respect to the *x* direction) while e^{-irx} and e^{-ikx} represent a particle moving to the left (with respect to the *x* direction). A particle inside the barrier will move only to the right but a particle to the left of the barrier may move either to the right (if "shot") or left (if reflected). The wave function Ψ and its first derivative were assumed to be continuous at $x = 0$.

Finally, the reflection coefficient as a function of E/V (for values of $E/V \geq 1$) was plotted and appears in the Appendix.

MOTIVATION

The quantum mechanical example of anti-tunneling is useful because it shows that subatomic and atomic particles behave differently from the classical mechanics model. Anti-tunneling shows that a particle possesses some chance of being reflected from a barrier; provided that barrier has less energy than the particle. This is analogous, in classical mechanics, to throwing a baseball with a great force at a window and having the baseball reflect off of it. The objective of this project was to find the probability of a particle being reflected from a barrier.

MATHEMATICAL DESCRIPTION AND SOLUTION APPROACH

The following two equations describe the motion of the wave:

$$\frac{h^2}{8\pi^2 m}\frac{d^2\Psi_1}{dx^2} = -E\Psi_1 \qquad x < 0, \tag{1}$$

$$\frac{h^2}{8\pi^2 m}\frac{d^2\Psi_2}{dx^2} = -(E - V)\Psi_2 \qquad x \geq 0, \tag{2}$$

where Ψ_1, and Ψ_2 are the wave functions of the particle introduced in the problem statement. The solution of these equations is given by

$$\Psi_1 = A_1 e^{irx} + B_1 e^{-irx} \tag{3}$$

$$\Psi_2 = A_2 e^{ikx} + B_2 e^{-ikx}. \tag{4}$$

Evaluating the first and second derivatives of Ψ_1 yields

$$\frac{d\Psi_1}{dx} = irA_1 e^{irx} - irB_1 e^{-irx} \tag{5}$$

$$\frac{d^2\Psi_1}{dx^2} = -r^2 A_1 e^{irx} - r^2 B_1 e^{-irx} \tag{6}$$

and evaluating the first and second derivatives of Ψ_2 gives

$$\frac{d\Psi_2}{dx} = ikA_2e^{ikx} - ikB_2e^{-ikx} \tag{7}$$

$$\frac{d^2\Psi_2}{dx^2} = -k^2A_2e^{ikx} - k^2B_2e^{-ikx} \tag{8}$$

Substitution of (3) and (6) into equation (1) gives

$$\left(\frac{\hbar^2}{2m}\right)\left(-r^2A_1e^{irx} - r^2B_1e^{-irx}\right) = -E\left(A_1e^{irx} + B_1e^{-irx}\right)$$

where $\hbar = h/2\pi$. Solving for r^2 yields

$$r^2 = \frac{2mE}{\hbar^2}\frac{\left(A_1e^{irx} + B_1e^{-irx}\right)}{\left(A_1e^{irx} + B_1e^{-irx}\right)} = \frac{2mE}{\hbar^2}$$

which implies that

$$r = \sqrt{\frac{2mE}{\hbar^2}}. \tag{9}$$

Similarly, substituting (4) and (8) into equation (2) and once again letting $\hbar = h/2\pi$ gives

$$\left(\frac{\hbar^2}{2m}\right)\left(-k^2A_2e^{ikx} - k^2B_2e^{-ikx}\right) = -(E-V)\left(A_2e^{ikx} + B_2e^{-ikx}\right),$$

and solving for k^2 results in

$$k^2 = \frac{2m(E-V)}{\hbar^2}\frac{\left(A_2e^{ikx} + B_2e^{-ikx}\right)}{\left(A_2e^{ikx} + B_2e^{-ikx}\right)} = \frac{2m(E-V)}{\hbar^2}$$

i.e.

$$k = \sqrt{\frac{2m(E-V)}{\hbar^2}}. \tag{10}$$

Since each $\Psi(x)$ and $\frac{d\Psi}{dx}$ are continuous at $x = 0$, (3) and (4) says that

$$A_1 + B_1 = \Psi_1(0) = \Psi_2(0) = A_2 + B_2 \tag{11}$$

and (5) and (6) says that

$$irA_1 - irB_1 = \frac{d\Psi_1}{dx}(0) = \frac{d\Psi_2}{dx}(0) = ikA_2 - ikB_2,$$

or simply that

$$A_1 - B_1 = \frac{k}{r}(A_2 - B_2). \tag{12}$$

However, $B_2 = 0$ since the particle is not traveling towards the left-hand *x*-direction after entering the barrier. Therefore, substituting $B_2 = 0$ into equations (11) and (12) yields,

$$A_1 - B_1 = \frac{k}{r}A_2 \qquad \text{and} \qquad A_1 + B_1 = A_2.$$

and solving this system of equations yields

$$A_1 = \frac{1}{2}A_2\left(1 + \frac{k}{r}\right) \tag{13}$$

$$B_1 = \frac{1}{2}A_2\left(1 - \frac{k}{r}\right) \tag{14}$$

Simplifying the expression of $\frac{k}{r}$ using (9) and (10) gives

$$\frac{k}{r} = \frac{\sqrt{\frac{2m(E-V)}{\hbar^2}}}{\sqrt{\frac{2mE}{\hbar^2}}} = \sqrt{\frac{2m\hbar^2(E-V)}{2m\hbar^2 E}} = \sqrt{\frac{E-V}{E}} = \sqrt{1 - \frac{V}{E}} = \sqrt{1 - \frac{1}{E/V}} \tag{15}$$

The reflection coefficient is defined as $\left(\frac{B_1}{A_1}\right)^2$. Equations (13), (14) and (5) imply that

$$\left(\frac{B_1}{A_1}\right)^2 = \left(\frac{\frac{1}{2}A_2\left(1-\frac{k}{r}\right)}{\frac{1}{2}A_2\left(1+\frac{k}{r}\right)}\right)^2 = \left(\frac{\left(1-\frac{k}{r}\right)}{\left(1+\frac{k}{r}\right)}\right)^2 = \left(\frac{\left(1-\sqrt{1-\frac{1}{E/V}}\right)}{\left(1+\sqrt{1-\frac{1}{E/V}}\right)}\right)^2. \quad (16)$$

A graph of the reflection coefficient vs. E/V appears in the Appendix.

DISCUSSION

The equation for the reflection coefficient (16) describes the probability of the particle being reflected from the barrier. The graph (see Appendix) helps to visualize how the chance of reflection related to E/V. As shown, the particle has a very high chance of being reflected when $E/V \approx 1$. This can also be explained by considering the limit of the function as E/V approaches one.

$$\lim_{\frac{E}{V}\to 1}\left(\frac{\left(1-\sqrt{1-\frac{1}{E/V}}\right)}{\left(1+\sqrt{1-\frac{1}{E/V}}\right)}\right)^2 = 1. \quad (17)$$

However, as the energy of the particle increases, the probability of the particle being reflected decreases at an exponential rate. This probability approaches 0 as E/V increases:

$$\lim_{\frac{E}{V}\to \infty}\left(\frac{\left(1-\sqrt{1-\frac{1}{E/V}}\right)}{\left(1+\sqrt{1-\frac{1}{E/V}}\right)}\right)^2 = 0. \quad (18)$$

This result is as expected. If the limit did not converge, there would be an unreasonably high probability that particles will be reflected off of the energy barrier.

Conclusion and Recommendations

After graphing the reflection coefficient of the particle (see Appendix), counterintuitive results were obtained. Even though the particle had more than enough energy to penetrate the barrier, it still had some small chance of being reflected. This discovery suggested that subatomic particles do not act in a manner described by classical physics and new models are required to describe their behaviors. The summary of this graph showed that the probability of the particle being reflected decreases exponentially as the ratio of E/V increases. One possible extension of this project would be to solve for the reflection coefficient considering the case where $V > E$.

Nomenclature

h = Planck's constant = $6.626 * 10^{-34} \left(\frac{\mathrm{m^2kg}}{\mathrm{s}}\right)$

$\hbar = \frac{\mathrm{h}}{2\pi} \left(\frac{\mathrm{m^2kg}}{\mathrm{s}}\right)$

m = the particle mass (kg)

E = the particle energy (J)

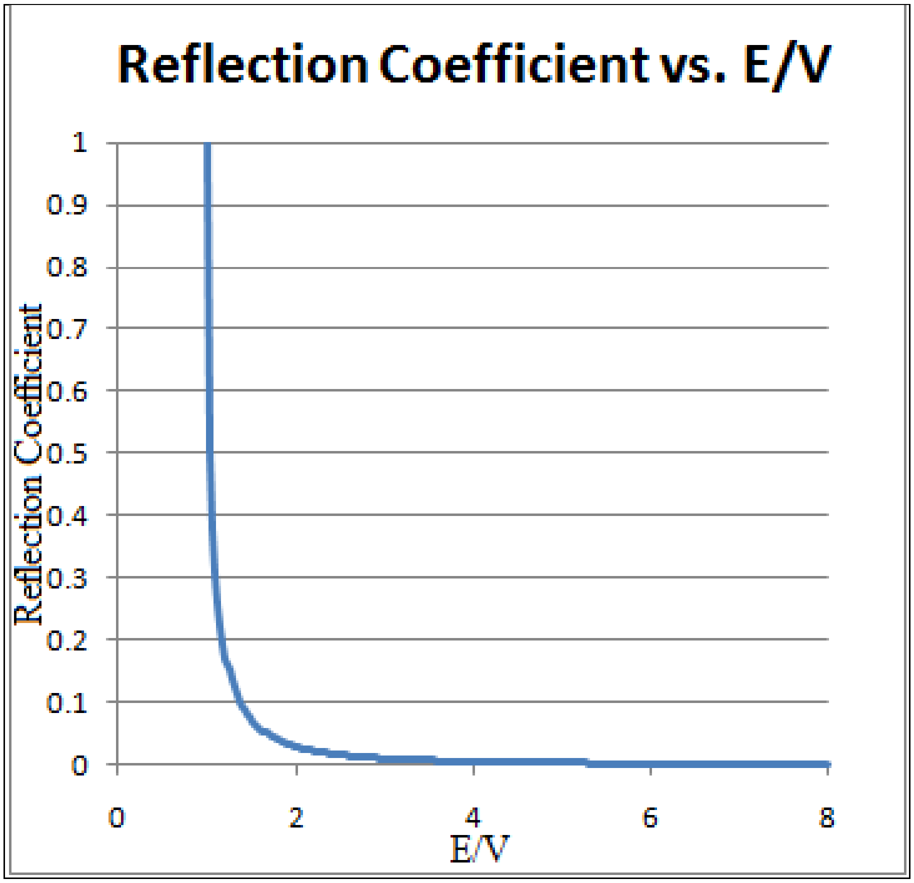
V = the potential height of the barrier (J)

Ψ = the wave function for the particle

Reference

Ferry, D. "Quantum Mechanics, An Introduction for Device Physicists and Electrical Engineers. Second Edition." Taylor & Francis Group, New York. (2001)

APPENDIX


Reflection Coefficient vs. E/V
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Reflection Coefficient
0
2
4
6
8
E/V