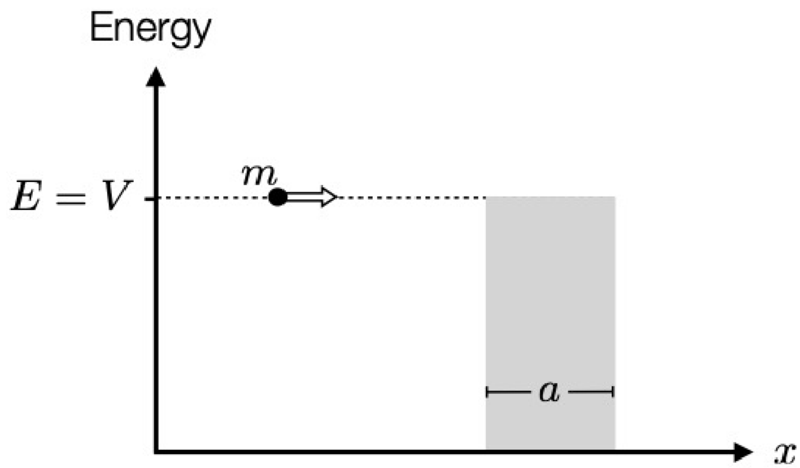
5. (Quantum Mechanics)

Starting with the time-independent Schrödinger equation, work out the fraction of incident particles transmitted through a rectangular one-dimensional potential barrier in the case shown below, where the energy E of the incident particles is equal to the barrier height V. Let the particles have mass m and let the barrier width be a.



Solution: *Solution by Jonah Hyman (jthyman@g.ucla.edu)*

The time-independent Schrödinger equation for a particle moving in one dimension is

$$H\psi(x) = E\psi(x) \tag{2}$$

where H is the Hamiltonian, E is the energy of the particle, and $\psi(x)$ is the wave function of the particle.

For a nonrelativistic particle, the Hamiltonian is given by

$$H = \frac{p^2}{2m} + V(x) \tag{3}$$

where $p^2/(2m)$ is the nonrelativistic kinetic energy and $V(x)$ is the potential. In this problem, the only feature of the potential is the constant-height barrier. In order to solve the problem in the simplest possible coordinate system, set $x = 0$ to be the left side of the barrier. In this coordinate system, the potential is given by

$$V(x) = \begin{cases} V & \text{for} \quad 0 \leq x \leq a \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

The definition of the quantum mechanical momentum operator in one dimension is

$$p = \frac{\hbar}{i}\frac{d}{dx} \tag{5}$$

Putting all this together, we get the Hamiltonian in all regions

$$H = \begin{cases} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V & \text{for} \quad 0 \leq x \leq a \\ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} & \text{otherwise} \end{cases} \tag{6}$$

To find the fraction of incident particles transmitted, we need to find the wave function everywhere. There are three regions in this problem:

- The left region, given by $x < 0$
- The center region, given by $0 \leq x \leq a$ (the barrier)
- The right region, given by $a < x$

In this case, we are given that the energy E is equal to V. Therefore, the time-independent Schrödinger equation (2) becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = V\,\psi \quad \text{for} \quad x < 0 \tag{7}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\,\psi = V\,\psi \quad \text{for} \quad 0 \leq x \leq a \tag{8}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = V\,\psi \quad \text{for} \quad a < x \tag{9}$$

Each of these equations needs to be solved separately. Fortunately, (7) and (9) are the same equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = V\,\psi$$

Rearranging, we get

$$\frac{d^2\psi}{dx^2} = -\frac{2mV}{\hbar^2}\,\psi$$
$$\frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{for} \quad k^2 \equiv \frac{2mV}{\hbar^2} > 0 \tag{10}$$

This is equivalent to the ordinary differential equation for simple harmonic motion $\frac{d^2\psi}{dx^2} + k^2\psi = 0$. The general solution to this differential equation is a sum of sines and cosines, or equivalently, a sum of complex exponentials. In this case, the complex exponentials will be easier to work with. With that in mind, let's write

$$\psi(x) = (\text{constant})\, e^{ikx} + (\text{constant})\, e^{-ikx} \tag{11}$$

There are two constants, which corresponds to the fact that this is a second-order differential equation. Setting different constants for the left and right regions, we can write general solutions for ψ_L and ψ_R:

$$\psi_L(x) = A\, e^{ikx} + B\, e^{-ikx} \quad \text{and} \quad \psi_R(x) = F\, e^{ikx} + G\, e^{-ikx} \quad \text{for} \quad k^2 \equiv \frac{2mV}{\hbar^2}$$

Now for the center region, governed by differential equation (8). We can simplify this equation to get

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\,\psi = V\,\psi$$
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = 0$$
$$\frac{d^2\psi}{dx^2} = 0 \tag{12}$$

To solve this second-order differential equation, recall that any linear function and any constant function have vanishing second derivative. Therefore, the solutions to $\frac{d^2\psi}{dx^2} = 0$ are sums of linear functions and constant functions:

$$\psi(x) = Cx + D$$

Combining our solutions for all three regions, we get the following general solution for $\psi(x)$:

$$\psi(x) = \begin{cases} A\, e^{ikx} + B\, e^{-ikx} & \text{for} \quad x < 0 \\ Cx + D & \text{for} \quad 0 < x < a \\ F\, e^{ikx} + G\, e^{-ikx} & \text{for} \quad a < x \end{cases}$$

Now it's time to apply the boundary conditions for this setup. The wave function is always required to be continuous. Its derivative is also always required to be continuous (unless there is a delta function in the potential, which there isn't here). This means that we require

$$\psi(x \to 0^-) = \psi(x \to 0^+) \quad \text{and} \quad \psi(x \to a^-) = \psi(x \to a^+) \quad \text{(continuity)}$$
$$\left.\frac{d\psi}{dx}\right|_{x\to 0^-} = \left.\frac{d\psi}{dx}\right|_{x\to 0^+} \quad \text{and} \quad \left.\frac{d\psi}{dx}\right|_{x\to a^-} = \left.\frac{d\psi}{dx}\right|_{x\to a^+} \quad \text{(continuity of derivative)}$$

Finally, we need to have a boundary condition at infinity. This condition comes from the fact that we want particles to be incident from only one side. In this case, we will set that to be the left side.

Note that a wave function of the form e^{ikx} represents a free particle moving to the right, while a wave function of the form e^{-ikx} represents a free particle moving to the left. This is because the time-evolution of a wave function $\psi(x)$ with energy E is given by

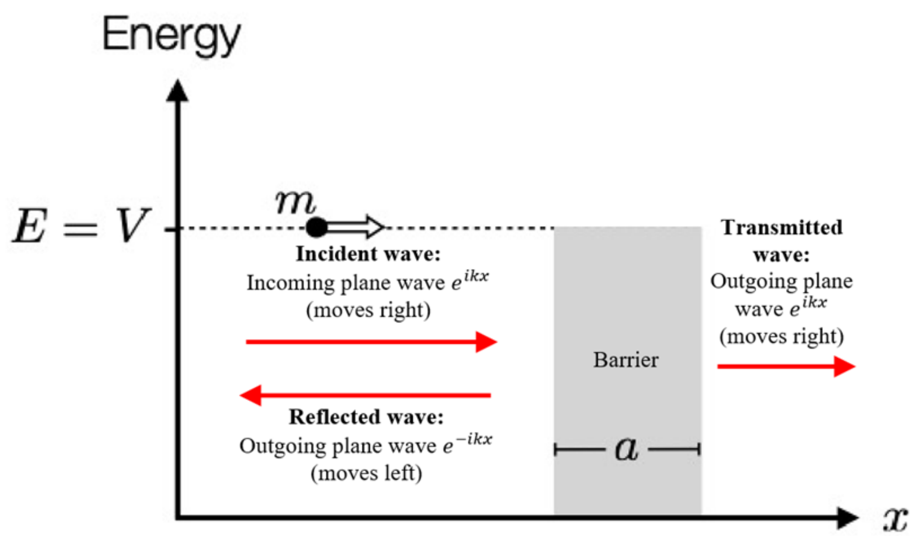
$$\psi(x,t) = \psi(x)e^{-i\omega t} \quad \text{for} \quad \omega \equiv \frac{E}{\hbar} \tag{13}$$

Therefore, a wave function of the form e^{ikx} time evolves as

$$\psi(t,x) = e^{i(kx-\omega t)} \tag{14}$$

which is the expression for a plane wave moving to the right. Similarly, we can show that a wave function of the form e^{-ikx} represents a plane wave moving to the left.

Since we only want particles to be incident from the left side of the barrier, we expect all particles on the right side of the barrier to be moving outward, i.e., to the right. (On the left side of the barrier, we expect particles to be moving both ways, since some of the particles reflect off the barrier.)



This means that we must have

$$\psi(x \to \infty) \propto e^{ikx}$$

Collecting the general form of the solution and the boundary conditions, we have

$$\psi(x) = \begin{cases} A\,e^{ikx} + B\,e^{-ikx} & \text{for} \quad x < 0 \\ Cx + D & \text{for} \quad 0 < x < a \\ F\,e^{ikx} + G\,e^{-ikx} & \text{for} \quad a < x \end{cases} \tag{15}$$

$$\psi(x \to 0^-) = \psi(x \to 0^+) \quad \text{and} \quad \psi(x \to a^-) = \psi(x \to a^+) \quad \text{(continuity)} \tag{16}$$

$$\left.\frac{d\psi}{dx}\right|_{x\to 0^-} = \left.\frac{d\psi}{dx}\right|_{x\to 0^+} \quad \text{and} \quad \left.\frac{d\psi}{dx}\right|_{x\to a^-} = \left.\frac{d\psi}{dx}\right|_{x\to a^+} \quad \text{(continuity of derivative)} \tag{17}$$

$$\psi(x \to \infty) \propto e^{ikx} \quad \text{(direction of incident wave)} \tag{18}$$

Boundary condition (18), the fact that the incident wave comes from the left, gives us

$$G = 0 \tag{19}$$

Boundary condition (16), the continuity of the wave function at $x = 0$ and $x = a$, gives us (applying $G = 0$ where applicable)

$$A + B = D \quad (\text{at } x = 0) \tag{20}$$

$$Ca + D = Fe^{ika} \quad (\text{at } x = a) \tag{21}$$

Boundary condition (17), the continuity of the derivative of wave function at $x = 0$ and $x = a$, gives us

$$ikA\,e^{ikx} - ikBe^{-ikx}\big|_{x=0} = C \tag{22}$$

$$ik(A - B) = C \quad (\text{at } x = 0) \tag{23}$$

and (applying $G = 0$ where applicable)

$$C = ikFe^{ikx}\big|_{x=a}$$

$$C = ikFe^{ika} \quad (\text{at } x = d) \tag{24}$$

To find the fraction of particles transmitted, we need to find F (which represents the strength of the transmitted plane wave) in terms of A (which represents the strength of the incident plane wave).

To start, we can eliminate C. Plugging (24) into (23) yields

$$ik(A - B) = ikFe^{ika}$$

$$A - B = Fe^{ika} \tag{25}$$

and plugging (24) into (21) yields

$$ikaFe^{ika} + D = Fe^{ika}$$

$$D = Fe^{ika}(1 - ika) \tag{26}$$

This allows us to eliminate the only other occurrence of D, in (20):

$$A + B = Fe^{ika}(1 - ika) \tag{27}$$

(25) and (27) are two equations for the unknowns B and F in terms of A. We can now add the two equations to one another to solve for F:

$$\begin{array}{cccccc} A & - & B & = & Fe^{ika} \\ A & + & B & = & Fe^{ika}(1 - ika) \\ \hline 2A & & & = & Fe^{ika}(2 - ika) \end{array}$$

This gives us

$$F = \frac{2}{2 - ika} e^{-ika}\,A \tag{28}$$

All that remains is to extract the fraction of incident particles transmitted (i.e. the transmission coefficient) from this information. The number of particles of a certain type (e.g. the number of incident particles, or the number of transmitted particles) is proportional to the probability of finding a particle of that type, which is equal to the absolute value squared of the wave function for particles of that type.

The wave function for incident particles (those to the left of the barrier, moving rightward toward the barrier) is

$$\psi_{\text{incident}}(x) = Ae^{ikx} \tag{29}$$

and the wave function for transmitted particles (those to the right of the barrier, moving rightward from the barrier) is

$$\psi_{\text{transmitted}}(x) = Fe^{ikx} \tag{30}$$

(We don't include the Be^{-ikx} term since that describes reflected particles, those to the left of the barrier, moving leftward away from the barrier.)

Therefore, the number of incident particles is proportional to

$$|\psi_{\text{incident}}(x)|^2 = |A|^2 \tag{31}$$

and the number of transmitted particles is proportional to

$$|\psi_{\text{transmitted}}(x)|^2 = |F|^2 \tag{32}$$

Since the left and right sides of the barrier have the same potential, the *fraction* of transmitted particles is therefore

$$\begin{aligned} T &= \frac{|\psi_{\text{transmitted}}(x)|^2}{|\psi_{\text{incident}}(x)|^2} \\ &= \frac{|F|^2}{|A|^2} \\ T &= \left| \frac{2}{2 - ika} e^{-ika} \right|^2 \quad \text{by our result for } F \text{ in terms of } A \text{ (28)} \end{aligned} \tag{33}$$

Taking the absolute value, we get

$$\begin{aligned} T &= \frac{4}{|2 - ika|^2} \\ &= \frac{4}{4 + (ka)^2} \\ T &= \frac{1}{1 + (ka/2)^2} \end{aligned} \tag{34}$$

Recall that k is defined by $k^2 \equiv \frac{2mV}{\hbar^2}$ (see (10)), so

$$\begin{aligned} \left(\frac{ka}{2}\right)^2 &= \frac{k^2 a^2}{4} \\ &= \frac{\frac{2mV}{\hbar^2} a^2}{4} \\ &= \frac{mVa^2}{2\hbar^2} \end{aligned}$$

Plugging this into (34), we get the fraction of particles transmitted as

$$\boxed{T = \frac{1}{1 + \frac{mVa^2}{2\hbar^2}}} \tag{35}$$