Quantum Mechanics

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> Lesson V March 5, 2019

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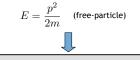


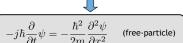
Scattering in one dimension

- Step potential
- Potential barrier and tunneling
- The ins and outs of tunneling

LAST CLASS WE SAW

 $E\psi = \hbar\omega\psi = -j\hbar\frac{\partial}{\partial t}\psi \qquad \qquad p_x\psi = \hbar k\psi = j\hbar\frac{\partial}{\partial x}\psi$





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Notation $\Rightarrow i = j$

.. The Free-Particle Schrodinger Wave Equation !

probability

$$P(x) = |\psi|^2 dx$$



Erwin Schrödinger (1887-1961) Image in the Public Domain

The Schrodinger Wave Equation

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

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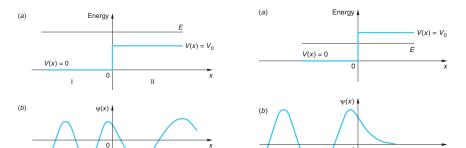
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Quantum Intuition

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

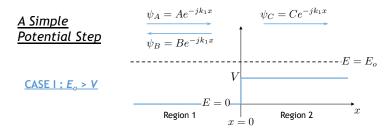




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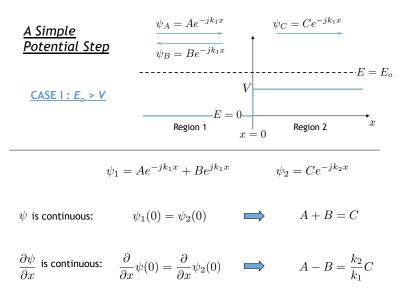
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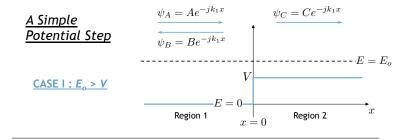


In Region 1:
$$E_o\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$
 $\implies k_1^2 = \frac{2mE_o}{\hbar^2}$

In Region 2:
$$(E_o - V) \psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \qquad \Longrightarrow \quad k_2^2 = \frac{2m \left(E_o - V\right)}{\hbar^2}$$



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$$\frac{B}{A} = \frac{1 - k_2/k_1}{1 + k_2/k_1} \qquad \frac{C}{A} = \frac{2}{1 + k_2/k_1} \qquad \Leftarrow \qquad \begin{cases} A + B = C \\ \\ \\ \\ \\ \\ \\ A - B = \frac{k_2}{k_1}C \end{cases}$$
$$= \frac{2k_1}{k_1 + k_2}$$

Quantum Electron Currents

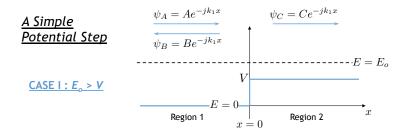
Given an electron of mass m

that is located in space with charge density $\left. \rho = q \left| \psi(x) \right|^2
ight.$

and moving with momentum $\, {\rm corresponding}$ to $\, < v > = \hbar k/m$

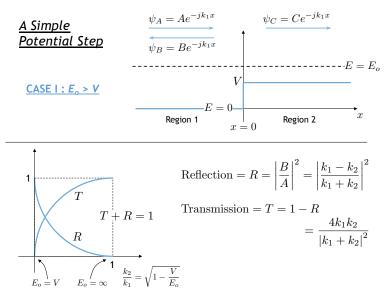
... then the current density for a single electron is given by

$$J = \rho v = q \left|\psi\right|^2 \left(\hbar k/m\right)$$



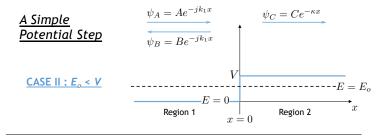
$$\begin{aligned} \text{Reflection} &= R = \frac{J_{reflected}}{J_{incident}} = \frac{J_B}{J_A} = \frac{|\psi_B|^2(\hbar k_1/m)}{|\psi_A|^2(\hbar k_1/m)} = \left|\frac{B}{A}\right|^2 \\ \text{Transmission} &= T = \frac{J_{transmitted}}{J_{incident}} = \frac{J_C}{J_A} = \frac{|\psi_C|^2(\hbar k_2/m)}{|\psi_A|^2(\hbar k_1/m)} = \left|\frac{C}{A}\right|^2 \frac{k_2}{k_1} \\ \frac{B}{A} &= \frac{1 - k_2/k_1}{1 + k_2/k_1} \qquad \frac{C}{A} = \frac{2}{1 + k_2/k_1} \end{aligned}$$

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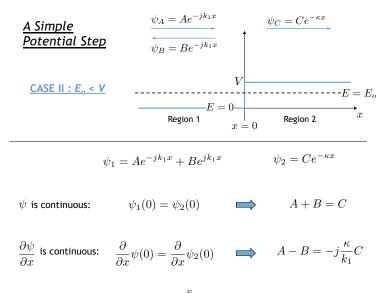


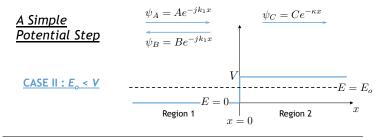
In Region 1:
$$E_o\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$
 $\implies k_1^2 = \frac{2mE_o}{\hbar^2}$

In Region 2:
$$(E_o - V)\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \implies \kappa^2 = \frac{2m(E_o - V)}{\hbar^2}$$

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$$\frac{B}{A} = \frac{1+j\kappa/k_1}{1-j\kappa/k_1} \qquad \qquad \frac{C}{A} = \frac{2}{1-j\kappa/k_1}$$

$$R = \left|\frac{B}{A}\right|^2 = 1 \qquad \qquad T = 0$$

Total reflection \rightarrow Transmission must be zero

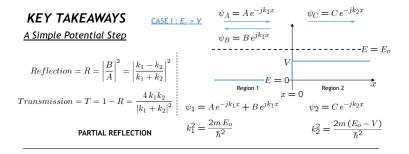
$$\label{eq:alpha} \left\{ \begin{matrix} A+B=C \\ \\ \\ \\ A-B=-j\frac{\kappa}{k_1}C \end{matrix} \right.$$

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$$R = |\frac{B}{A}|^2 = 1$$

$$T = 0$$

$$\psi_1 = A e^{-jk_1x}$$

$$\psi_B = B e^{jk_1x}$$

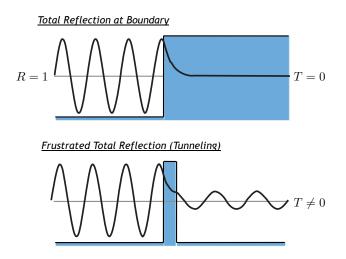
$$\psi_C = C e^{-\kappa x}$$

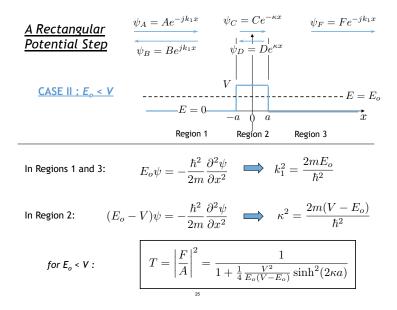
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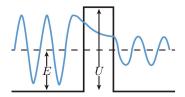
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Quantum Tunneling Through a Thin Potential Barrier





<u>A Rectangular</u> Potential Step



for $E_o < V$:

$$T = \left|\frac{F}{A}\right|^2 = \frac{1}{1 + \frac{1}{4}\frac{V^2}{E_o(V - E_o)}\sinh^2(2\kappa a)}$$

$$\sinh^2(2\kappa a) = \left[e^{2\kappa a} - e^{-2\kappa a}\right]^2 \approx e^{-4\kappa a}$$
$$T = \left|\frac{F}{A}\right|^2 \approx \frac{1}{1 + \frac{1}{4}\frac{V^2}{E_o(V - E_o)}}e^{-4\kappa a}$$

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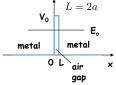
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Example: Barrier Tunneling

• Let's consider a tunneling problem:

An electron with a total energy of $E_o= 6 \text{ eV}$ approaches a potential barrier with a height of $V_0 = 12 \text{ eV}$. If the width of the barrier is L = 0.18 nm, what is the probability that the electron will tunnel through the barrier?

~



$$T = \left|\frac{F}{A}\right|^2 \approx \frac{16E_o(V - E_o)}{V^2}e^{-2\kappa L}$$

$$\kappa = \sqrt{\frac{2m_e}{\hbar^2}(V - E_o)} = 2\pi \sqrt{\frac{2m_e}{\hbar^2}(V - E_o)} = 2\pi \sqrt{\frac{6 \mathrm{eV}}{1.505 \mathrm{eV} \mathrm{-nm}^2}} \approx 12.6 \ \mathrm{nm}^{-1}$$

$$T = 4e^{-2(12.6 \text{ nm}^{-1})(0.18 \text{ nm})} = 4(0.011) = 4.4\%$$

Question: What will T be if we double the width of the gap?

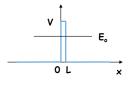
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Multiple Choice Questions

Consider a particle tunneling through a barrier:

- 1. Which of the following will increase the likelihood of tunneling?
 - a. decrease the height of the barrier
 - b. decrease the width of the barrier
 - c. decrease the mass of the particle



- 2. What is the energy of the particles that have successfully "escaped"?
 - a. < initial energy
 - b. = initial energy
 - c. > initial energy

Although the *amplitude* of the wave is smaller after the barrier, no energy is lost in the tunneling process

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Schrodinger Equations

Key to solving for the wave function of a particle hitting a potential barrier is finding the **Schrodinger equations** which describe the system. First, define the energy potential, V(x), of the system as this:

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

Writing the wave function of the particle as $\psi_1(x)$ for x < 0, $\psi_2(x)$ for 0 < x < a, and $\psi_3(x)$ for x > a, the **Schrodinger equations** for x < 0, 0 < x < a, and x > a are respectively:

$$E\psi_1(x) = -rac{\hbar^2}{2m}rac{d^2}{dx^2}\psi_1(x)$$
 (2)

$$E\psi_2(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_2(x) + V_0 \psi_2(x)$$
(3)

$$E\psi_3(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_3(x)$$
(4)

This can be simplified, considering the wavenumbers, k_1 and k_2 , of the wave function for inside and outside the barrier respectively. Since $k_1^2 = 2mE/\hbar^2$ and $k_2^2 = 2m(E - V_0)/\hbar^2$, this can be said of the wave function of a particle with $E \ge V_0$.

$$0 = \frac{d^2}{dx^2} \psi_1(x) + k_1^2 \psi_1(x)$$
(5)

$$0 = \frac{d^2}{dx^2} \psi_2(x) + k_2^2 \psi_2(x) \tag{6}$$

$$0 = \frac{d^2}{dx^2}\psi_3(x) + k_1^2\psi_3(x)$$
(7)

Notice, however that if $E < V_0$, k_2 is imaginary and thus no longer an observable. By convention therefore, κ , defined by $\kappa^2 = 2m(V_0 - E)/\hbar^2$, is used instead for $E < V_0$. The differential equations defining the wave function of a particle with insufficient energy are thus:

$$0 = \frac{d^2}{dx^2}\psi_1(x) + k_1{}^2\psi_1(x) \tag{8}$$

$$0 = \frac{d^2}{dx^2}\psi_2(x) - \kappa^2\psi_2(x)$$
(9)

$$0 = \frac{\frac{d^2}{dx^2}}{dx^2}\psi_3(x) + k_1^2\psi_3(x)$$
(10)

If There Is Sufficient Energy

For $E \ge V_0$, to find the wave function of the particle, equations (5), (6), and (7) must be solved. These are homogeneous second-order linear differential equations and have the following general solutions:

$$\psi_1(x) = A e^{r_A x} + B e^{r_B x} \tag{11}$$

$$\psi_2(x) = C e^{r_C x} + D e^{r_D x} \tag{12}$$

$$\psi_3(x) = F e^{r_F x} + G e^{r_G x} \tag{13}$$

where A, B, C, D, F, and G are constants and $r_A = r_F$ and $r_B = r_G$ are the two solutions to the equation $r^2 + k_1^2 = 0$ while r_C and r_D are the two solutions to the equation $r^2 + k_2^2 = 0$.

 $\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \tag{14}$

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \tag{15}$$

$$\psi_3(x) = F e^{ik_1 x} + G e^{-ik_1 x} \tag{16}$$

tice, considering **Euler's formula**, that Ae^{ik_1x} , Ce^{ik_2x} , and Fe^{ik_1x} represent waves travelling in the positive ection while Be^{-ik_1x} , De^{-ik_2x} , and Ge^{-ik_1x} represent waves travelling in the negative direction. Since reflection by e^{ik_1x} is conceivable, it is possible to have wave components travelling in the negative direction for x < a, but are is no reason to have waves doing so for x > a. Thus, G = 0.

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \tag{17}$$

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \tag{18}$$

$$\psi_3(x) = F e^{ik_1 x} \tag{19}$$

solve for B and F in relation to A, impose these four boundary conditions to ensure that the wave function is a ooth curve as $x \to 0$ and as $x \to a$:

$$egin{aligned} &\lim_{x o 0^-}\psi_1(x) &=\lim_{x o 0^+}\psi_2(x)\ &\lim_{x o 0^-}rac{d}{dx}\psi_1(x) &=\lim_{x o 0^+}rac{d}{dx}\psi_2(x)\ &\lim_{x o a^-}rac{d}{y}\psi_2(x) &=\lim_{x o a^+}rac{d}{y}x(x)\ &\lim_{x o a^-}rac{d}{dx}\psi_2(x) &=\lim_{x o a^+}rac{d}{dx}\psi_3(x) \end{aligned}$$

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$$A + B = C + D \tag{20}$$

$$ik_1A - ik_1B = ik_2C - ik_2D$$
 (21)

$$Ce^{ik_2a} + De^{-ik_2a} = Fe^{ik_1a} (22)$$

$$ik_2 C e^{ik_2 a} - ik_2 D e^{-ik_2 a} = ik_1 F e^{ik_1 a}$$
⁽²³⁾

$$k_1A + k_1B = k_1C + k_1D$$
(24)
$$k_1A - k_1B = k_2C - k_2D$$
(25)
$$k_2Ce^{ik_2a} + k_2De^{-ik_2a} = k_2Fe^{ik_1a}$$
(26)
$$k_2Ce^{ik_2a} - k_2De^{-ik_2a} = k_1Fe^{ik_1a}$$
(27)

$$2k_1A = (k_1 + k_2)C + (k_1 - k_2)D$$
⁽²⁸⁾

$$2k_1B = (k_1 - k_2)C + (k_1 + k_2)D$$
⁽²⁹⁾

$$2k_2Ce^{ik_2a} = (k_1 + k_2)Fe^{ik_1a} \tag{30}$$

$$2k_2 D e^{-ik_2 a} = (k_2 - k_1) F e^{ik_1 a}$$
(31)

To solve for F in relation to A, consider equations (28), (30), and (31).

$$2k_1A = \frac{(k_1 + k_2)^2}{2k_2}Fe^{i(k_1 - k_2)a} - \frac{(k_1 - k_2)^2}{2k_2}Fe^{i(k_1 + k_2)a}$$
(32)

$$4k_1k_2e^{-ik_1a}A = (k_1 + k_2)^2Fe^{-ik_2a} - (k_1 - k_2)^2Fe^{ik_2a}$$
(33)

Using **Euler's formula** to expand e^{-ik_2a} and e^{ik_2a} , the following can be derived:

$$4k_1k_2e^{-ik_1a}A = \left(-2ik_1^2\sin k_2a + 4k_1k_2\cos k_2a - 2ik_2^2\sin k_2a\right)F$$
(34)

$$F = \frac{2k_1k_2e^{-ik_1a}A}{2k_1k_2\cos k_2a - i\left(k_1^2 + k_2^2\right)\sin k_2a}$$
(35)

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To solve for B in relation to A, consider equations (29), (30), and (31).

$$2k_1B = \frac{k_1^2 - k_2^2}{2k_2} F e^{i(k_1 - k_2)a} - \frac{k_1^2 - k_2^2}{2k_2} F e^{i(k_1 + k_2)a}$$
(36)

$$\frac{4k_1k_2e^{-ik_1a}B}{k_1^2 - k_2^2} = \left(e^{-ik_2a} - e^{ik_2a}\right)F \tag{37}$$

Using **Euler's formula** to expand e^{-ik_2a} and e^{ik_2a} , the following can be derived:

$$\frac{2k_1k_2e^{-ik_1a}B}{-i\left(k_1^2-k_2^2\right)\sin k_2a} = F$$
(38)

Comparing equations (35) and (38), B is solved for in relation to A.

$$B = \frac{-i(k_1^2 - k_2^2)\sin(k_2a)A}{2k_1k_2\cos k_2a - i(k_1^2 + k_2^2)\sin k_2a}$$
(39)

Considering equations (30) and (31) alongside equation (35), C and D can also be solved for in relation to A, but since only A, B, and F are needed to calculate the reflection and transmission coefficients, the derivations of C and D are omitted here. In order to find the reflection and transmission coefficients, the wave function must be first written in terms of its incident, reflected, and transmitted components, $\psi_i(x)$, $\psi_r(x)$, and $\psi_t(x)$ respectively.

$$\psi_i(x) = A e^{ik_1 x} \tag{40}$$

$$\psi_r(x) = Be^{-ik_1x} \tag{41}$$

$$\psi_t(x) = F e^{ik_1 x} \tag{42}$$

The reflection and transmission coefficients, R and T respectively, are defined as follows:

$$R = -\frac{j_r}{j_i}$$
(43)
$$T = \frac{j_t}{j_i}$$
(44)

where j_i , j_r , and j_t are the incident, reflected, and transmitted **probability currents** respectively.

$$R = -\frac{\psi_r(x)\frac{d}{dx}\psi_r^{*}(x) - \psi_r^{*}(x)\frac{d}{dx}\psi_r(x)}{\psi_i(x)\frac{d}{dx}\psi_i^{*}(x) - \psi_i^{*}(x)\frac{d}{dx}\psi_i(x)}$$

$$T = \frac{\psi_t(x)\frac{d}{dx}\psi_t^{*}(x) - \psi_t^{*}(x)\frac{d}{dx}\psi_t(x)}{\psi_i(x)\frac{d}{dx}\psi_i^{*}(x) - \psi_i^{*}(x)\frac{d}{dx}\psi_i(x)}$$
(45)

$$R = \frac{|B|^2}{|A|^2}$$
(47)
$$T = \frac{|F|^2}{|A|^2}$$
(48)

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Applying the solutions for B and F found in equations (39) and (35) respectively gives:

$$R = \frac{(k_1^2 - k_2^2)^2 \sin^2 k_2 a}{4k_1^2 k_2^2 \cos^2 k_2 a + (k_1^2 + k_2^2)^2 \sin^2 k_2 a}$$
(49)
$$T = \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 \cos^2 k_2 a + (k_1^2 + k_2^2)^2 \sin^2 k_2 a}$$
(50)

$$R = \frac{\left(k_1^2 - k_2^2\right)^2 \sin^2 k_2 a}{4k_1^2 k_2^2 + \left(k_1^2 - k_2^2\right)^2 \sin^2 k_2 a}$$
(51)

$$T = \frac{4k_1^2k_2^2}{4k_1^2k_2^2 + (k_1^2 - k_2^2)^2\sin^2 k_2 a}$$
(52)

$$R = \left[\frac{4k_1^2 k_2^2}{(k_1^2 - k_2^2)^2 \sin^2 k_2 a} + 1\right]^{-1}$$
(53)
$$T = \left[\frac{(k_1^2 - k_2^2)^2 \sin^2 k_2 a}{4k_1^2 k_2^2} + 1\right]^{-1}$$
(54)

Interestingly contrary to classical mechanics, quantum mechanics suggests that the particle may actually be reflected by the potential barrier, despite having a total energy of equal or greater value than V_0 .

If There Is Insufficient Energy

For $E < V_0$, equations (8), (9), and (10) must be solved to find $\psi_1(x)$, $\psi_2(x)$, and $\psi_3(x)$. To do this, follow the methodology employed in the previous section, **"If There Is Sufficient Energy"**. The solutions of equations (8), (9), and (10) are identical to those of (5), (6), and (7) respectively save for the use of $i\kappa$ in the place of k_2 .

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \tag{55}$$

$$\psi_2(x) = Ce^{-\kappa x} + De^{\kappa x} \tag{56}$$

$$\psi_3(x) = F e^{ik_1 x} \tag{57}$$

Applying the same boundary conditions as in the previous section and manipulating algebra in the same manner, it can also be found that:

$$2ik_1A = (ik_1 - \kappa)C + (ik_1 + \kappa)D \tag{58}$$

$$2ik_1 B = (ik_1 + \kappa)C + (ik_1 - \kappa)D$$
(59)

$$2\kappa C e^{-\kappa a} = (\kappa - ik_1) F e^{ik_1 a} \tag{60}$$

$$2\kappa D e^{\kappa a} = (ik_1 + \kappa) F e^{ik_1 a} \tag{61}$$

To solve for F in relation to A, consider equations (58), (60), and (61).

$$2ik_1 A = -\frac{(ik_1 - \kappa)^2}{2\kappa} F e^{(ik_1 + \kappa)a} + \frac{(ik_1 + \kappa)^2}{2\kappa} F e^{(ik_1 - \kappa)a}$$
(62)

$$4ik_1\kappa e^{-ik_1a}A = -(ik_1 - \kappa)^2 F e^{\kappa a} + (ik_1 + \kappa)^2 F e^{-\kappa a}$$
(63)

$$4ik_1\kappa e^{-ik_1a}A = \left[\left(k_1^2 - \kappa^2\right)\left(e^{\kappa a} - e^{-\kappa a}\right) + 2ik_1\kappa\left(e^{\kappa a} + e^{-\kappa a}\right)\right]F\tag{64}$$

$$F = \frac{2ik_1\kappa e^{-ik_1a}A}{\left(k_1^2 - \kappa^2\right)\sinh\kappa a + 2ik_1\kappa\cosh\kappa a} \tag{65}$$

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(In case you are unfamiliar with hyperbolic functions, $\sinh u = (e^u - e^{-u})/2$ is the hyperbolic sine function and $\cosh u = (e^u + e^{-u})/2$ is the hyperbolic cosine function.) To solve for B in relation to A, consider equations (59), (60), and (61).

$$2ik_1B = \frac{k_1^2 + \kappa^2}{2\kappa} F e^{(ik_1 + \kappa)a} - \frac{k_1^2 + \kappa^2}{2\kappa} F e^{(ik_1 - \kappa)a}$$
(66)

$$\frac{4ik_1\kappa e^{-ik_1a}B}{k_1^2+\kappa^2} = Fe^{\kappa a} - Fe^{-\kappa a}$$
(67)

$$\frac{2ik_1\kappa e^{-ik_1a}B}{\left(k_1^2+\kappa^2\right)\sinh\kappa a} = F \tag{68}$$

Comparing equations (65) and (68), B is solved for in relation to A.

$$B = \frac{(k_1^2 + \kappa^2)\sinh(\kappa a)A}{(k_1^2 - \kappa^2)\sinh\kappa a + 2ik_1\kappa\cosh\kappa a}$$
(69)

As in the previous section, the wave function written in terms of its incident, reflected, and transmitted components is:

$$\psi_i(x) = A e^{ik_1 x} \tag{70}$$

$$\psi_r(x) = B e^{-ik_1 x} \tag{71}$$

$$\psi_t(x) = F e^{ik_1 x} \tag{72}$$

Furthermore, the reflection and transmission coefficients, derivable using the same method as in the previous section, are again given by:

$$R = \frac{|B|^2}{|A|^2}$$
(73)
$$T = \frac{|F|^2}{|A|^2}$$
(74)

$$R = \frac{(k_1^2 + \kappa^2)^2 \sinh^2 \kappa a}{(k_1^2 - \kappa^2)^2 \sinh^2 \kappa a + 4k_1^2 \kappa^2 \cosh^2 \kappa a}$$
(75)
$$T = \frac{4k_1^2 \kappa^2}{(k_1^2 - \kappa^2)^2 \sinh^2 \kappa a + 4k_1^2 \kappa^2 \cosh^2 \kappa a}$$
(76)

$$R = \frac{\left(k_{1}^{2} + \kappa^{2}\right)^{2} \sinh^{2} \kappa a}{\left(k_{1}^{2} + \kappa^{2}\right)^{2} \sinh^{2} \kappa a + 4k_{1}^{2} \kappa^{2}}$$

$$T = \frac{4k_{1}^{2} \kappa^{2}}{\left(k_{1}^{2} + \kappa^{2}\right)^{2} \sinh^{2} \kappa a + 4k_{1}^{2} \kappa^{2}}$$
(78)

$$R = \left[\frac{4k_1^2 \kappa^2}{\left(k_1^2 + \kappa^2\right)^2 \sinh^2 \kappa a} + 1\right]^{-1}$$
(79)
$$T = \left[\frac{\left(k_1^2 + \kappa^2\right)^2 \sinh^2 \kappa a}{4k_1^2 \kappa^2} + 1\right]^{-1}$$
(80)

Contrary to classical expectations which would suggest that the particle has zero probability of travelling beyond x = 0, quantum mechanics asserts that the particle has a non-zero probability of tunneling through the rectangular potential barrier, despite having a total energy less than V_0 . This phenomenon marks a major difference between quantum and classical mechanics.