EXERCISE 21

Tunneling through a rectangular potential barrier

1. Solve the time-independent Schrödinger equation,
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)\,,$$
for a particle encountering a rectangular potential barrier, where the potential function is given by
$$V(x) = \begin{cases} V_0 & \text{if} \quad -a < x < a \\ 0 & \text{otherwise} \end{cases}\,.$$
Consider the scenario in which the particle's energy is less than the height of the barrier, i.e.
$$0 < E < V_0\,.$$

2. Using the obtained solution, demonstrate that the probability of the particle tunneling through the barrier is given by
$$T = \left[\cosh^2(2k'a) + \left(\frac{k^2 - k'^2}{2kk'}\right)^2 \sinh^2(2k'a)\right]^{-1}\,,$$
where
$$k = \frac{\sqrt{2mE}}{\hbar} \quad \text{and} \quad k' = \frac{\sqrt{2m(V_0 - E)}}{\hbar}\,.$$

3. Show that if $k'a \gg 1$, or, equivalently, if
$$V_0 - E \gg \frac{\hbar^2}{2ma^2}\,,$$
the formula for the tunneling probability can be approximated by
$$T \simeq 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)\exp\left(-\frac{4a}{\hbar}\sqrt{2m(V_0 - E)}\right)\,.$$
This approximation explicitly shows the exponential sensitivity of the tunneling probability to the barrier width, which forms the basis for the operation of the scanning tunneling microscope (STM).

Solution

1. Let us consider separately three spatial regions: $x < -a$, $-a < x < a$, and $x > a$.

   For $\boxed{x < -a}$ the Schrödinger equation reads

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

   or

   $$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0\,,$$

   where

   $$k = \frac{\sqrt{2mE}}{\hbar}\,.$$

   The general (up to an overall constant multiplier) solution can be written as

   $$\psi(x) = e^{ikx} + Be^{-ikx}\,. \tag{1}$$

   Here, just as in Exercise 19, the amplitude of the incoming plane wave is chosen to be one. The amplitude B of the reflected plane wave is yet to be determined.

   For $\boxed{-a < x < a}$ the Schrödinger equation reads

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

   or

   $$\frac{d^2\psi(x)}{dx^2} - k'^2\psi(x) = 0\,,$$

   where

   $$k' = \frac{\sqrt{2m(V_0 - E)}}{\hbar}\,.$$

   The general solution is

   $$\psi(x) = Ce^{k'x} + De^{-k'x}\,, \tag{2}$$

   where C and D are some yet-unknown constants.

   Finally, for $\boxed{x > a}$ the Schrödinger equation again assumes the free-particle form,

   $$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0\,.$$

   Keeping only the outgoing plane wave, propagating from left to right, away from the potential barrier, we have

   $$\psi(x) = Fe^{ikx}\,. \tag{3}$$

Here, F is the transmission (or tunneling) amplitude that remains to be determined.

The amplitudes B, C, D, and F are determined by ensuring that the function $\psi(x)$ remains smooth across the entire x-axis. To achieve this, we must impose matching conditions that guarantee the continuity and differentiability of $\psi(x)$ at $x = -a$ and $x = a$.

At $\boxed{x = -a}$ we have

$$\left\{ \begin{array}{l} \psi(-a-0) = \psi(-a+0) \\ \frac{d\psi}{dx}(-a-0) = \frac{d\psi}{dx}(-a+0) \end{array} \right. \quad \Longrightarrow \quad \left\{ \begin{array}{l} e^{-ika} + Be^{ika} = Ce^{-k'a} + De^{k'a} \\ ike^{-ika} - ikBe^{ika} = k'Ce^{-k'a} - k'De^{k'a} \end{array} \right.$$

As in Exercise 19, we add -0 (respectively, $+0$) to the argument of a function to indicate that the function is evaluated immediately to the left (respectively, to the right) of that point.

At $\boxed{x = a}$ we have

$$\left\{ \begin{array}{l} \psi(a-0) = \psi(a+0) \\ \frac{d\psi}{dx}(a-0) = \frac{d\psi}{dx}(a+0) \end{array} \right. \quad \Longrightarrow \quad \left\{ \begin{array}{l} Ce^{k'a} + De^{-k'a} = Fe^{ika} \\ k'Ce^{k'a} - k'De^{-k'a} = ikFe^{ika} \end{array} \right.$$

In summary, we obtain the following system of four linear equations that determine B, C, D, and F:

$$-e^{ika}B + e^{-k'a}C + e^{k'a}D = e^{-ika} \tag{4}$$

$$ike^{ika}B + k'e^{-k'a}C - k'e^{k'a}D = ike^{-ika} \tag{5}$$

$$e^{k'a}C + e^{-k'a}D - e^{ika}F = 0 \tag{6}$$

$$k'e^{k'a}C - k'e^{-k'a}D - ike^{ika}F = 0 \tag{7}$$

This system can be solved using any standard method, such as straightforward elimination. The result is given by

$$B = -i\left(k'^2 + k^2\right)\sinh(2k'a)e^{-i2ka}Z \tag{8a}$$

$$C = k(k' + ik)e^{-ka'-ika}Z \tag{8b}$$

$$D = k(k' - ik)e^{k'a-ika}Z \tag{8c}$$

$$F = 2kk'e^{-i2ka}Z \tag{8d}$$

with

$$Z = \frac{1}{2kk'\cosh(2k'a) + i\left(k'^2 - k^2\right)\sinh(2k'a)}\,.$$

Equations (1), (2), (3), and (8) constitute the solution to the Schrödinger equation for $E < V_0$.

2. The particle's energy is lower than the barrier height. Classically, there can be no transmission through the barrier. Quantum mechanically, however, the transmission probability (in this context referred to as tunneling probability) can be non-zero. The transmission (or tunneling) probability is determined by the squared modulus of the transmission amplitude,

$$\begin{aligned} T &= |F|^2 \\ &= |2kk'e^{-i2ka}Z|^2 \\ &= 4k^2k'^2 Z^* Z \\ &= \frac{4k^2k'^2}{4k^2k'^2\cosh^2(2k'a) + \left(k'^2 - k^2\right)^2 \sinh^2(2k'a)} \,, \end{aligned}$$

or

$$\boxed{T = \frac{1}{\cosh^2(2k'a) + \left(\frac{k^2-k'^2}{2kk'}\right)^2 \sinh^2(2k'a)}}$$

3. If $k'a \gg 1$, then

$$\begin{aligned} \cosh(2k'a) &= \frac{1}{2}\left(e^{2k'a} + e^{-2k'a}\right) \simeq \frac{e^{2k'a}}{2} \,, \\ \sinh(2k'a) &= \frac{1}{2}\left(e^{2k'a} - e^{-2k'a}\right) \simeq \frac{e^{2k'a}}{2} \,, \end{aligned}$$

and, consequently,

$$T \simeq \frac{4e^{-4k'a}}{1 + \left(\frac{k^2-k'^2}{2kk'}\right)^2} = \frac{4e^{-4k'a}}{\left(\frac{k^2+k'^2}{2kk'}\right)^2} = \left(\frac{4kk'}{k^2+k'^2}\right)^2 e^{-4k'a} \,.$$

Expressed in terms of energy E, the tunneling probability reads

$$T \simeq \left(\frac{4\sqrt{E(V_0-E)}}{E + (V_0 - E)}\right)^2 \exp\left(-\frac{4a}{\hbar}\sqrt{2m(V_0-E)}\right) \,,$$

or

$$\boxed{T \simeq 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)\exp\left(-\frac{4a}{\hbar}\sqrt{2m(V_0-E)}\right)}$$