Even Solutions to the Finite-Depth Square Well

\[ a := 1 \quad \text{Half width of the square well} \]

\[ A := 1 \quad \text{Normalization constant} \]

\[ z_0 := 7 \quad \text{Depth of the well } (a \text{ times sqrt}(2mV_0)/h) \]

\[ \kappa(z) := \sqrt{z_0^2 - z^2} \quad \text{Decay constant for the exponential tails} \]

\[ B(z) := A \cdot \cos(z) \cdot e^{\kappa(z) \cdot a} \quad \text{Normalization of the exponential tails} \]

\[ \psi(x, z) := \begin{cases} x < -a, B(z) \cdot e^{\kappa(z) \cdot x}, & \text{if } x < a, A \cdot \cos\left(\frac{z}{a}\right), B(z) \cdot e^{-\kappa(z) \cdot x} \end{cases} \quad \text{Wave Function} \]

\[ f_1(z) := \tan(z) \]

\[ f_2(z) := \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \quad f(z) := f_1(z) - f_2(z) \quad \text{Function to solve for eigenvalues} \]

\[ z = k \cdot a \quad k = \text{wave number} \]

Graphical Solution for Eigenvalues

For these parameters there are three solutions. The wave functions are plotted below.

Note that from the graph it is obvious that no matter how small \( z_0 \) is, there will always be at least one solution.
Solve numerically for the 1st eigenvalue

First Even Solution

Solve numerically for the 2nd eigenvalue

Second Even Solution

Solve numerically for the 3rd eigenvalue

Third Even Solution
\[ V(x) := \text{if} \left( x < a, 0, \text{if} \left( x < -z_0^2, 0 \right) \right) \]

\[ z_1 = 1.373 \quad z_2 = 4.089 \quad z_3 = 6.616 \]
Reflection From a Step Potential

\( h_{\text{bar}} := \frac{6.6 \times 10^{-28}}{2 \pi} \quad \text{m} := 10^{-31} \)  
\( \text{Units: time in ps, distance in nm, mass in kg} \)

\( a := 0.002 \quad V_0 := 10^{-20} \)  
Barrier width and potential, and the energy

\( r := 0.5 \quad E := r V_0 \)

\( V(x) := \text{if}(x < 0, 0, 1) \)  
Potential barrier, with arbitrary height, for plotting

\( k_0 := \left[ \frac{2m E}{h_{\text{bar}}} \right]^{1/2} = 301.048 \)  
Wave number outside of the barrier region

\( \kappa_0 := \frac{i \text{if}(E < V_0 \cdot 1, -1)}{h_{\text{bar}}} \sqrt{\frac{2m (V_0 - E)}{E}} \)  
Decay coefficient within the barrier region

\( \kappa_0 \cdot a = 0.602 \)

Wave eigenfunction for a plane wave incident from the left with unit amplitude:

\( B(k, \kappa) := \frac{(\kappa + i k)}{\kappa - i k} \quad C(k, \kappa) := 1 + B(k, \kappa) \)

\( \psi(x, k, \kappa) := \text{if}(x < 0, e^{i k x} + B(k, \kappa) e^{-i k x}, C(k, \kappa) e^{-\kappa x}) \)

\( P(x) := \bar{\psi}(x, k_0, \kappa_0) \psi(x, k_0, \kappa_0) \)  
Probability density

\( R := \left( \left| B(k_0, \kappa_0) \right| \right)^2 \)  
\( R = 1 \)  
Reflection coefficient

\( T := \text{if} \left( E > V_0 \cdot \sqrt{\frac{E - V_0}{E}} \right) \left( \left| C(k_0, \kappa_0) \right| \right)^2, 0 \)  
\( T = 0 \)  
Transmission coefficient

\( R + T = 1 \)  
Check that they add up to unity.

![Probability Density (not normalized)](image-url)
Now, use the eigenfunctions calculated above to simulate a wave packet incident on the barrier. The behavior is rather different in this case, because there is a significant range of wave numbers included. In fact, the upper end of the range included below extends above the well, so the transmission is not entirely from tunneling. On the other hand, the lower end of the range has an exponentially lower tunneling probability.

\[ x_0 := -30 \cdot a = -0.06 \quad \sigma_x := 2a = 4 \times 10^{-3} \quad \text{Initial position and gaussian width of the wave packet} \]

\[ \sqrt{\frac{2mV_0}{\hbar}} = 425.746 \quad \text{Wave number for an energy right at the top of the potential barrier} \]

\[ \sigma_k := \frac{1}{2} \sigma_x = 125 \quad \bar{k}_0 = 301.048 \quad \text{Width and central value in k space (momentum space)} \]

\[ v_0 := \frac{\hbar \bar{k}_0}{m} \quad t_0 := \frac{-x_0}{v_0} = 1.897 \times 10^{-7} \quad \text{Packet speed, and elapsed time when it hits the barrier.} \]

\[ \phi(k) := \left(2\pi\sigma_k^2\right)^{-1/4} e^{-\frac{1}{4} \left(k-k_0\right)^2} \cdot e^{-i(k-k_0)x_0} \quad \text{This makes a gaussian distribution of wave numbers designed to make a gaussian-shaped wave packet centered around } x_0 \text{ at time 0 and moving to the right with speed } v_0. \]

\[ \int_{-\infty}^{\infty} \phi(k) \cdot \overline{\phi(k)} \, dk = 1 \quad \text{Check the normalization} \]
Now make a wave function by summing (integrating) eigenfunctions for all values of $k$ within 4-sigma of the peak. The integral is done numerically, which is rather time consuming, but the resulting video requires only about 1/2 hour of CPU time to make on a notebook PC.

$$E_0 := \frac{2mV_0}{\hbar^2} = 425.746$$

$$\kappa(k) := \text{if}(k > E_0, -1, 1) \sqrt{\frac{2mV_0}{\hbar^2} - k^2} \quad \kappa(k_0) = 301.048$$

$$\omega(k) := \frac{\hbar k^2}{2m} \quad \omega(k_0) = 4.76 \times 10^7$$

$$\Psi(x, t) := \frac{1}{\sqrt{2\pi}} \int_{k_0 - 4\sigma_k}^{k_0 + 4\sigma_k} \phi(k) \cdot \psi(x, k, \kappa(k)) \cdot e^{-i \omega(k) \cdot t} dk$$

$$\rho(x, t) := \left( |\Psi(x, t)| \right)^2$$

![Probability Density Graph]
Probability Density

\[ \rho(x, t_0) \]

\[ \frac{1}{16a} V(x) \]

Probability Density

\[ \rho(x, 2t_0) \]

\[ \frac{1}{16a} V(x) \]