

5.6: Solving the 1D Semi-Infinite Square Well

Imagine a particle trapped in a one-dimensional well of length L . Inside the well there is no potential energy. However, the “right-hand wall” of the well (and the region beyond this wall) has a finite potential energy. This means that it is possible for the particle to escape the well if it had enough energy.

Again, since this potential is a piece-wise function, Schrödinger’s equation must be solved in the three regions separately.

In the region $x < 0$, we have already seen that since the potential is infinite there is no chance of finding the particle in this region. Thus, $\Psi = 0$ in this region.

In the region $0 < x < L$, the equation and solution should look familiar:

$$\begin{aligned} -\frac{\hbar}{2m} \frac{d^2}{dx^2} \Psi(x) + U(x)\Psi(x) &= E\Psi(x) \\ -\frac{\hbar}{2m} \frac{d^2}{dx^2} \Psi(x) + (0)\Psi(x) &= E\Psi(x) \\ -\frac{\hbar}{2m} \frac{d}{dx^2} \Psi(x) &= E\Psi(x) \\ \frac{d^2}{dx^2} \Psi(x) &= -\frac{2mE}{\hbar^2} \Psi(x) \end{aligned} \quad (5.6.1)$$

The general solution to this equation is

$$\Psi(x) = A \sin(kx) + B \cos(kx) \text{ with } k = \sqrt{\frac{2mE}{\hbar^2}} \quad (5.6.2)$$

In order for this solution to be continuous with the solution for $x < 0$, the coefficient B must equal zero. Thus,

$$\Psi(x) = A \sin(kx) \quad (5.6.3)$$

In the region $x > L$, the equation is:

$$\begin{aligned} -\frac{\hbar}{2m} \frac{d^2}{dx^2} \Psi(x) + U(x)\Psi(x) &= E\Psi(x) \\ -\frac{\hbar}{2m} \frac{d^2}{dx^2} \Psi(x) &= (E - U)\Psi(x) \\ \frac{d^2}{dx^2} \Psi(x) &= \frac{2m(U - E)}{\hbar^2} \Psi(x) \end{aligned} \quad (5.6.4)$$

The general solution is:

$$\Psi(x) = Ce^{aX} + De^{-aX} \text{ with } \alpha = \sqrt{\frac{2m(U - E)}{\hbar^2}} \quad (5.6.5)$$

Since this region contains the point $x = +\infty$, C must equal zero or the wavefunction will diverge. Therefore,

$$\Psi(x) = De^{-aX} \quad (5.6.6)$$

The wave function, and the derivative of the wave function, must be continuous across the boundary at $x = L$. Forcing continuity leads to:

$$\begin{aligned} \Psi(x = L^-) &= \Psi(x = L^+) \\ A \sin(kL) &= De^{-aL} \end{aligned} \quad (5.6.7)$$

and forcing the continuity of the derivative leads to:

$$\begin{aligned} \Psi(x = L^-) &= \Psi(x = L^+) \\ kA \cos(kL) &= -\alpha De^{-aL} \end{aligned} \quad (5.6.8)$$

Substituting the first equation into the second equation yields:

$$\begin{aligned} & kA \cos(kL) = -\alpha (A \sin(kL)) \\ & \tan(kL) = -\frac{k}{\alpha} \end{aligned}$$

$$\sqrt{\frac{2mE}{\hbar^2}} L = -\frac{\sqrt{2mE}}{\sqrt{U-E}}$$

This last result is a transcendental equation for the allowed energy levels. If the potential energy and width of the well are known, the allowed energy levels can be determined by using a solver or graphing the function.

The 1D Semi-Infinite Well

Determine the allowed energy levels for a proton trapped in a semi-infinite square well of width 5.0 fm and depth 60 MeV.

Applying the previous result:

$$\tan\left(\sqrt{\frac{2mE}{\hbar^2}} L\right) = -\sqrt{\frac{E}{U-E}}$$

$$\tan\left(\sqrt{\frac{2(938 \text{ MeV})(5.0 \text{ fm})^2 E}{(194.7 \text{ MeV fm})^2}}\right) = -\sqrt{\frac{E}{60-E}}$$

$$\tan\left(\sqrt{1.204 E}\right) = -\sqrt{\frac{E}{60-E}}$$

with E in MeV.

The solutions to this equation, which represent the allowed energy levels for the proton, are 6.53, 25.75, and 55.08 MeV.

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