Appendix 4.1
Alternate Solution to the Infinite Square Well with Symmetric Boundary Conditions

In this problem, a particle of mass $m$ confined by a potential energy which has a position dependence described by the figure above. The potential energy is infinite for region I, where $x < -L/2$ and for region III, where $x > +L/2$, but is zero in region II, where $-L/2 \leq x \leq +L/2$. We must find the solution to Schrödinger's time-independent equation in these three regions.

Schrödinger's time-independent equation

\[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + V(x) \psi(x) = E \psi(x)\]  \hspace{1cm} (0.1)

can be written in the form

\[\frac{\partial^2}{\partial x^2} \psi(x) = -\frac{2m}{\hbar^2} [E - V(x)] \psi(x)\] \hspace{1cm} (0.2)

where

\[k = \sqrt{\frac{2m}{\hbar^2} [E - V(x)]}\] \hspace{1cm} (0.4)

Now in region I and III where $V(x) > E$ for any energy, $k$ is obviously imaginary. To make the imaginary nature of $k$ more explicit, we will write $k = i\kappa$, where $\kappa = \sqrt{\frac{2m}{\hbar^2} [V(x) - E]}$ is real, and the equation above becomes

\[\frac{\partial^2}{\partial x^2} \psi(x) = +\kappa^2 \psi(x)\] \hspace{1cm} (0.5)
The general solution to this differential equation is simple — it must be of the form
\[ \psi(x) = Ae^{\lambda x} \] (0.6)
so that we have
\[ \lambda^2 Ae^{\lambda x} = + \kappa^2 Ae^{\lambda x} \] (0.7)
so that \( \lambda = \pm \kappa \), giving the general solution (the sum of the two possible solutions with appropriate arbitrary constants)
\[ \psi(x) = A e^{+\kappa x} + B e^{-\kappa x} \] (0.8)
The time-dependent solution of the Schrodinger equation for the case where \( V(x) > E \) is, therefore,
\[ \Psi(x,t) = [A e^{+\kappa x} + B e^{-\kappa x}]e^{-i\omega t} \] (0.9)
In the case of the infinite square well, where \( V(x) = \infty \), \( \kappa = \infty \), giving
\[ \Psi(x,t) = [A e^{+\infty} + B e^{-\infty}]e^{-i\omega t} \] (0.10)
The second term goes to zero, but the first term blows up unless we require \( A = 0 \)! In such a case, we require the wave function to be zero everywhere in region I and region III. This means that the solution inside the well must go to zero at the boundaries.

Now let's look at the solution in the region where \( V(x) = 0 \), and \( k = \sqrt{\frac{2mE}{h^2}} \). Again the general solution to the differential equation must be of the form
\[ \psi(x) = Ae^{\lambda x} \] (0.11)
giving
\[ \lambda^2 Ae^{\lambda x} = - k^2 Ae^{\lambda x} \] (0.12)
so that \( \lambda = \pm ik \). The general solution to this equation must be
\[ \psi(x) = A e^{+ikx} + B e^{-ikx} \] (0.13)
The time-dependent solution is, therefore,
\[ \Psi(x,t) = [A e^{+ikx} + B e^{-ikx}]e^{-i\omega t} \] (0.14)
or
\[ \Psi(x,t) = A e^{+i(kx+\omega t)} + B e^{-i(kx+\omega t)} \] (0.15)

Now using Euler's relationship we can write this last equation in the form
\[ \Psi(x,t) = A [\cos(kx - \omega t) + i \sin(kx - \omega t)] + B[\cos(kx + \omega t) - i \sin(kx + \omega t)] \] (16)
where we have used the fact that $\cos(-x) = \cos(x)$ and $\sin(-x) = -\sin(x)$. Simplifying, we obtain

$$\Psi(x,t) = A \cos(kx - \omega t) + B \cos(kx + \omega t)$$

$$+ i[A \sin(kx - \omega t) - B \sin(kx + \omega t)]$$

(0.17)

In both the real and imaginary parts of this equation, we have two sinusoidal waves moving in opposite directions. The first term represents a real cosine wave moving in the $+x$ direction, while the second term represents such a wave moving in the $-x$ direction. This can be seen by observing a point on the wavefront where the phase, $\phi = kx \pm \omega t$ is equal to zero. Thus, the solution to Schrodinger's equation in the well is the solution of sinusoidal waves which are traveling in opposite directions, and interfering with each other.

The only wave functions which are allowed, however, are ones which go to zero at the boundaries of the well, i.e., at $x = \pm L/2$. Both the real and the imaginary parts of the wavefunction must go to zero at the boundary. At the boundary where $x = +L/2$, we have

$$A \cos(kL/2 - \omega t) + B \cos(kL/2 + \omega t) = 0$$

(0.18)

and

$$A \sin(kL/2 - \omega t) - B \sin(kL/2 + \omega t) = 0$$

(0.19)

While at the boundary where $x = -L/2$, we have

$$A \cos(-kL/2 - \omega t) + B \cos(-kL/2 + \omega t) = 0$$

(0.20)

and

$$A \sin(-kL/2 - \omega t) - B \sin(-kL/2 + \omega t) = 0$$

(0.21)

This can be more compactly written in terms of the equation

$$\Psi(x,t) = [ Ae^{+ikx} + Be^{-ikx} ] e^{-i\omega t}$$

(0.22)

Since the boundary conditions must be satisfied at all times, we require the term in brackets to go to zero when $x = +L/2$, and when $x = -L/2$, or

$$[ Ae^{+ikL/2} + Be^{-ikL/2} ] = 0$$

(0.23)

and

$$[ Ae^{-ikL/2} + Be^{+ikL/2} ] = 0$$

(0.24)

Solving for $A$ in both equations gives two different solutions

$$A = -Be^{\pm ikL}$$

(0.25)
both of which must be valid, so

\[-Be^{ikL} = -Be^{-ikL}\]  

\[
\cos(kL) + i \sin(kL) = \cos(kL) - i \sin(kL)
\]  

\[
\sin(kL) = -\sin(kL)
\]  

which can only be true if

\[
\sin(kL) = 0 \Rightarrow kL = n\pi \Rightarrow k = \frac{n\pi}{L}
\]

Applying this condition to both of the equations implied by Equ. 1.25 gives

\[
A = -B[\cos(n\pi) + i \sin(n\pi)] = -B[\cos(n\pi) - i \sin(n\pi)]
\]

which, since \(\sin(n\pi) = 0\), reduces to

\[
A = -B \cos(n\pi)
\]

This equation gives two different results for \(A\), depending upon the value of \(n\): for even \(n\), \(A = -B\), and for odd \(n\), \(A = B\). This means we have two sets of solutions:

1. For odd \(n\)

\[
\Psi(x,t) = A \left[ e^{+ikx} + e^{-ikx} \right] e^{-i\omega t} = A'(t) \cos(kx)
\]

\[
\Psi_{\text{odd}}(x,t) = A'(t) \cos(n\pi x/L)
\]

where \(A'(t) = (A/2)e^{-i\omega t}\)

2. For even \(n\)

\[
\Psi(x,t) = A \left[ e^{+ikx} - e^{-ikx} \right] e^{-i\omega t} = A'(t) \sin(kx)
\]

\[
\Psi_{\text{even}}(x,t) = A'(t) \sin(n\pi x/L)
\]

where \(A'(t) = (A/2i)e^{-i\omega t}\). Note that the solution where \(n = 0\) gives the null wavefunction, which we interpret as no solution.

The energy of the particle of mass \(m\) confined to the well is found using Equ. 0.0 and Equ. 0.0, to be

\[
E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 (n\pi/L)^2}{2m} = n^2 \left[ \frac{\hbar^2 \pi^2}{2mL^2} \right] = n^2 E_1
\]  

The solutions to the wave equation are shown in blue in Figure 2.1 for the first four values of the quantum number \(n\). These solutions are plotted on a line which represents the energy of that particular state in terms of \(E_1\). Plotted in red is the probability density...
\[ P(x, t) = P(x) \text{ given by} \]

\[ P(x, t) = \Psi^*(x, t)\Psi(x, t) = \left| \Psi(x, t) \right|^2 \quad (0.35) \]

\[ P(x, t) = P(x) = \begin{cases} 
\cos^2\left(\frac{n\pi x}{L}\right) & n \text{ odd} \\
\sin^2\left(\frac{n\pi x}{L}\right) & n \text{ even} 
\end{cases} \quad (0.36) \]

Since we define the probability in terms of the square of the absolute magnitude of the wavefunction, the time dependent terms of a particular eigenfunction cancel so that the probability density of an eigenfunction is time independent! This is a direct consequence of the fact that the solution to Schrodinger's equation can be written as a time-dependent part times a position-dependent part.