PHY140Y

22 Particle in a One Dimensional Box

22.1 Overview

- Schrödinger's Equation for a Particle in a Box
- Solutions

22.2 Schrödinger's Equation for a One Dimensional Box

We are going to use as a concrete example of how to use Schrödinger's equation a simple system – that of a particle with mass m confined inside a 1-dimensional box of length L. This is not as uninteresting an example as you might think, because when we extend this to a 3-dimensional box, we actually are talking about the quantum mechanics of an ideal gas.[1]

In order to solve for the wave function $\psi(x)$, we need to write down the correct potential energy function and identify the boundary conditions.

22.2.1 Potential Energy and Boundary Conditions

For this case, we are going to assume that the particle experiences NO forces on it while in the box, so that means $U(x)$ should be a constant anywhere in the box (*i.e.*, for $x \in (0, L)$). However, we need to keep the particle confined to the box, so we therefore make the potential energy infinite for $x \leq 0$ and for $x \geq L$. This gives the box "walls." For convenience, we will set $U(x) = 0$ for $x \in (0, L)$. This potential is illustrated in Fig. 1.

The boundary conditions on $\psi(x)$ will be set by what we know about the particle's motion. In particular, we know that the particle will never be found outside the box, so that at the edges of the box we must have

$$\psi(0) = 0 \quad \text{and} \quad \psi(L) = 0. \tag{1}$$

The other criterion we can employ is that the probability density we get from the wave function, $P(x) \equiv |\psi(x)|^2$, is normalized so that the probability of finding the particle somewhere in the box is unity:

$$\int_0^L |\psi(x)|^2 \, dx = 1. \tag{2}$$

[1] We won't get this far in this course, but you will have plenty of opportunity to study this in second year QM and Thermal Physics.

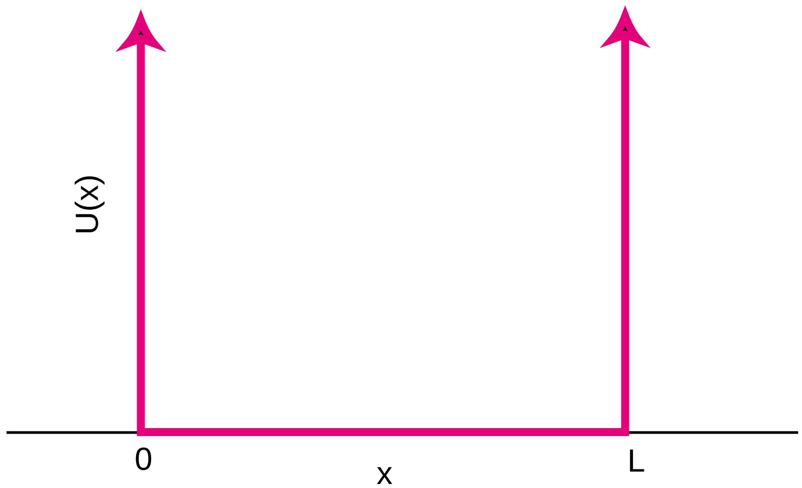

Figure 1: The potential energy function for a particle in a 1-D box.

22.3 Solutions to Schrödinger's Equations

With these conditions in mind, we can now solve Schrödinger's equation for $x \in (0, L)$:

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi(x) &= E\psi(x) && (3) \\ \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} &= E\psi(x) && (4) \\ \Rightarrow \frac{d^2\psi}{dx^2} &= -\left(\frac{2mE}{\hbar^2}\right)\psi(x). && (5) \end{aligned}$$

This is just the differential equation for a simple harmonic oscillator, which has the general solution

$$\psi(x) = A\sin(kx) + B\cos(kx), \qquad (6)$$

where k can be determined by substituting this into the differential equation:

$$\begin{aligned} k^2 &= \left(\frac{2mE}{\hbar^2}\right) && (7) \\ \Rightarrow k &= \frac{\sqrt{2mE}}{\hbar}. && (8) \end{aligned}$$

If we now apply the boundary condition $\psi(0) = 0$, we find

$$\begin{aligned} \psi(0) &= A\sin(0) + B\cos(0) = B && (9) \\ \Rightarrow B &= 0. && (10) \end{aligned}$$

If we now apply the boundary condition $\psi(L) = 0$, we find

$$\begin{aligned} \psi(L) &= A\sin(kL) && (11) \\ \Rightarrow A\sin(kL) &= 0 && (12) \\ \Rightarrow kL &= n\pi,\ n = 1, 2, 3, \ldots && (13) \end{aligned}$$

This implies that k can take on an infinite number of discrete values, denoted by

$$k_n = \frac{n\pi}{L}, \; n = 1, 2, 3, \ldots \tag{14}$$

Thus, the solution to the wave function is

$$\psi_n(x) = A_n \sin\left(n\pi x/L\right), \; n = 1, 2, 3, \ldots \tag{15}$$

To determine the constants A_n, we require the resulting wave function to be normalized. This means that

$$\begin{aligned}
1 &= \int_0^L |\psi_n(x)|^2 \, dx && (16)\\
&= A_n^2 \int_0^L \sin^2\left(n\pi x/L\right) dx && (17)\\
&= A_n^2 \int_0^{n\pi} \sin^2 \eta \, \left(\frac{L}{n\pi}\right) d\eta && (18)\\
&= A_n^2 \left(\frac{L}{\pi}\right) \int_0^{\pi} \sin^2 \eta \; d\eta && (19)\\
&= A_n^2 \left(\frac{L}{2}\right) && (20)\\
\Rightarrow A_n &= \sqrt{\frac{2}{L}} && (21)
\end{aligned}$$

where we have made a change of variable in the third line, $\eta \equiv n\pi x/L$, and have noted that the integral over $n\pi$ is n times the integral over π. Thus, the final form for the wave function can be one of the solutions

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(n\pi x/L\right), \; n = 1, 2, 3, \ldots \tag{22}$$

We'll examine the behaviour of these and their implications in the next lecture.