

Lecture Notes: January 13, Fri, Class 3

Schrodinger Equation Expressions for a Particle in 1-D Finite and 1-D Infinite Potential Wells and 3-D Infinite Potential Well



Objectives:

- Write Schrodinger Equations for bound states such as infinite and finite potential wells. Describe quantized energy states and wave functions for infinite and finite potential wells.
- Express the time-independent Schrodinger Equation for a particle in a 3-dimensional infinite well situation using (x, y, z) coordinates. Describe quantized energy states and wave functions. Understand energy degeneracies.

We have the time-independent Schrodinger Equation:

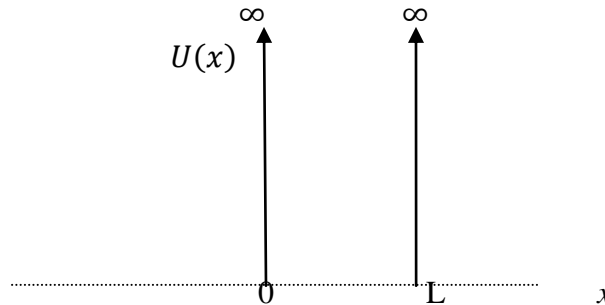
$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + U(x) \psi(x) = E \psi(x) \quad (e2.1)$$

Bound States represent cases when a particle's wave function is limited to a finite region of space by the potential energy, $U(x)$. We will consider wave functions and energies three such cases:

- Infinite Well where $U(x) =$ 
- Finite Well where $U(x) =$ 

2.1. Infinite Well

$$U(x) = \begin{cases} \infty & x \leq 0 \\ 0 & 0 < x < L \\ \infty & x \geq L \end{cases}$$



Where $x \leq 0$, wave functions CANNOT exist since the potential is infinity. $\rightarrow \psi_{x \leq 0}(x) = 0$

Where $x \geq L$, wave functions CANNOT exist since the potential is infinity $\rightarrow \psi_{x \geq L}(x) = 0$

Where $0 < x < L$, put $U(x) = 0$ into the time-independent Schrodinger Equation (e2.1),

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = E \psi(x) \quad (e2.2)$$

$$\frac{\partial^2 \psi(x)}{\partial x^2} = \frac{-2mE}{\hbar^2} \psi(x) = -k^2 \psi(x) \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}} \quad (e2.3)$$

Since the wave function has to be confined inside the infinite well, we can consider $\sin(kx)$ or $\cos(kx)$ that satisfy (e2.2) as $\psi_{0 < x < L}(x)$.

BUT, since $\psi(x)$ needs to be continuous which means

- $\psi_{x \leq 0}(x = 0) = 0 \rightarrow$ We take only $\sin(kx)$ for $\psi_{0 < x < L}(x)$ (drop $\cos(kx)$)
- $\psi_{x \geq L}(x = L) = 0 \rightarrow \psi_{0 < x < L}(x = L) = \sin(kL) = 0$ gives energy quantization rules

$$kL = \sqrt{\frac{2mE}{\hbar^2}} L = n\pi \quad \text{where } n = 1, 2, 3, \text{ etc.} \quad (\text{e2.4})$$

$$E = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad \text{Energy quantization} \quad (\text{e2.5})$$

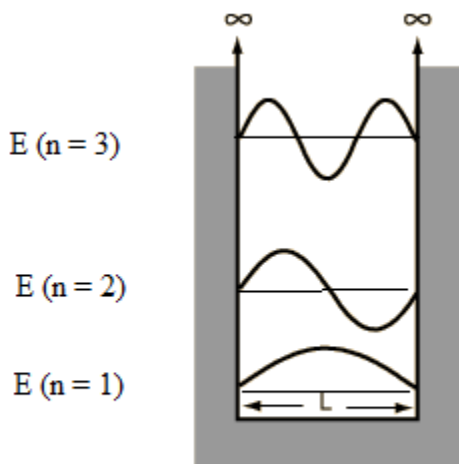
- Normalization

$$\psi_{0 < x < L}(x) = A \sin(kx) = A \sin\left(\frac{n\pi x}{L}\right)$$

$$\int_0^L |\psi_{0 < x < L}(x)|^2 dx = 1 = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = A^2 \frac{L}{2} \rightarrow A = \sqrt{\frac{2}{L}} \quad (\text{e2.6})$$

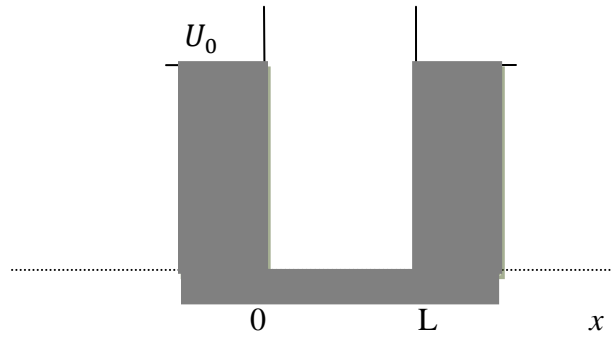
THEREFORE,

- Wave function: $\psi_{0 < x < L}(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$
- Energy $E = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$



2.2. Finite Well

$$U(x) = \begin{cases} U_0 & x \leq 0 \\ 0 & 0 < x < L \\ U_0 & x \geq L \end{cases}$$



where $0 < x < L$, $\psi_{0 < x < L} = Ae^{ikx} + Be^{-ikx}$ where $k = \sqrt{\frac{2mE}{\hbar^2}}$

where $x \leq 0$, $\psi_{x < 0}$ should decay exponentially as x moves below zero $= Ce^{\alpha x}$

$$\text{where } \alpha = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

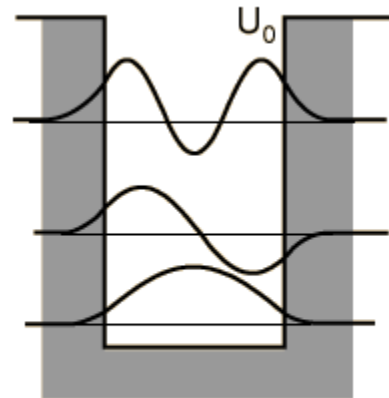
where $x \geq L$, $\psi_{x \geq L}$ should decay exponentially as x moves above $L = De^{-\alpha x}$

$$\text{where } \alpha = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

Since $\psi(x)$ should be continuous everywhere, the following conditions should be met:

- $\psi_{x \leq 0}(x = 0) = \psi_{0 < x < L}(x = 0)$
- $\frac{d\psi_{x \leq 0}}{dx} \Big|_{x=0} = \frac{d\psi_{0 < x < L}}{dx} \Big|_{x=0}$
- $\psi_{0 < x < L}(x = L) = \psi_{x \geq L}(x = L)$
- $\frac{d\psi_{0 < x < L}}{dx} \Big|_{x=L} = \frac{d\psi_{x \geq L}}{dx} \Big|_{x=L}$
- $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = (\text{normalization condition})$

This means, there are five equations to be solved for A, B, C, and D. An additional parameter has to obey these relationships. That additional parameter is k (therefore E). Not all energy values will meet all five equations.



2.3. Schrodinger Equation in three dimensions

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t} \rightarrow \frac{-\hbar^2}{2m} \nabla^2 \Psi(\vec{x}, t) + U(\vec{x})\Psi(\vec{x}, t) = i\hbar \frac{\partial \Psi(\vec{x}, t)}{\partial t}$$

In (x, y, z) coordinates, $\vec{x} = (x, y, z)$, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

The time-dependent Schrodinger Equation is:

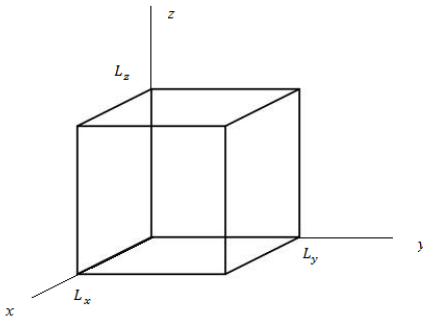
$$\frac{-\hbar^2}{2m} \nabla^2 \Psi(\vec{x}, t) + U(\vec{x})\Psi(\vec{x}, t) = i\hbar \frac{\partial \Psi(\vec{x}, t)}{\partial t} \quad (\text{e2.7})$$

$$\text{Normalization: } \int |\Psi(\vec{x}, t)|^2 dV = 1$$

The time-independent Schrodinger Equation is:

$$\frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{x}) + U(\vec{x})\psi(\vec{x}) = E \psi(\vec{x}) \quad (\text{e2.8})$$

2.4. The 3D Infinite Well



$$U(\vec{x}) = \begin{cases} 0 & 0 < x < L_x, 0 < y < L_y, 0 < z < L_z \\ \infty & \text{otherwise} \end{cases}$$

The 3D infinite well problem is an extension of the 1D infinite well problem in all three directions, because we can separate wave functions as

$$\psi(\vec{x}) = F(x)G(y)H(z) \quad (\text{e2.9})$$

If we put (e2.9) into (e2.8), we get

$$\frac{1}{F(x)} \frac{\partial^2 F(x)}{\partial x^2} + \frac{1}{G(y)} \frac{\partial^2 G(y)}{\partial y^2} + \frac{1}{H(z)} \frac{\partial^2 H(z)}{\partial z^2} = -\frac{2mE}{\hbar^2} \quad (\text{e2.10})$$

$$\begin{cases} \frac{d^2 F(x)}{dx^2} = C_x F(x) \rightarrow F(x) = A_x \sin \frac{n_x \pi x}{L_x} \\ \frac{d^2 G(y)}{dy^2} = C_y G(y) \rightarrow G(y) = A_y \sin \frac{n_y \pi y}{L_y} \\ \frac{d^2 H(z)}{dz^2} = C_z H(z) \rightarrow H(z) = A_z \sin \frac{n_z \pi z}{L_z} \end{cases} \quad (\text{e2.11})$$

Put (e2.11) into (e2.10)

$$-\frac{n_x^2 \pi^2}{L_x^2} - \frac{n_y^2 \pi^2}{L_y^2} - \frac{n_z^2 \pi^2}{L_z^2} = -\frac{2mE}{\hbar^2} \rightarrow E = \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right) \frac{\pi^2 \hbar^2}{2m} \quad (\text{e2.12}) \rightarrow \text{Energy Quantized!}$$

- Lowest Energy State is $(n_x, n_y, n_z) = (1, 1, 1)$
 - $E_{(1,1,1)} = \left(\frac{1^2}{L_x^2} + \frac{1^2}{L_y^2} + \frac{1^2}{L_z^2} \right) \frac{\pi^2 \hbar^2}{2m}$
 - $\psi_{(1,1,1)} = A \sin \frac{\pi x}{L_x} \sin \frac{\pi y}{L_y} \sin \frac{\pi z}{L_z}$

Degeneracy occurs when different wave functions have the same energy.

When $L_x = L_y = L_z = L$

We can see that

- $E = 3 \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) \rightarrow E_{(1,1,1)} \rightarrow$ One wave function $\psi_{(1,1,1)} = A \sin \frac{\pi x}{L} \sin \frac{\pi y}{L} \sin \frac{\pi z}{L}$
(nondegenerate)
- $E = 6 \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) \rightarrow E_{(2,1,1)} = E_{(1,2,1)} = E_{(1,1,2)}$

$$\rightarrow 3 \text{ wave functions } \begin{cases} \psi_{(2,1,1)} = A \sin \frac{2\pi x}{L} \sin \frac{\pi y}{L} \sin \frac{\pi z}{L} \\ \psi_{(1,2,1)} = A \sin \frac{\pi x}{L} \sin \frac{2\pi y}{L} \sin \frac{\pi z}{L} \\ \psi_{(1,1,2)} = A \sin \frac{\pi x}{L} \sin \frac{\pi y}{L} \sin \frac{2\pi z}{L} \end{cases}$$

(degenerate)

Degeneracy = 3 (# of different wave functions that correspond to the same energy)