

*Notes on Selected topics to accompany Sakurai's  
"Modern Quantum Mechanics"*

Raghunathan Ramakrishnan  
ramakrishnan@tifrh.res.in

Prepared for the course QM1 for Physicists at  
Tata Institute of Fundamental Research Hyderabad Hyderabad  
500046, India

---

*Series solution method for particle-in-a-box*

*Problem*

Determine the energy levels and normalized wavefunctions of a particle in a potential box. The potential energy of the particle is  $V = \infty$  for  $x < 0$  and  $x > a$ , and  $V = 0$  for  $0 < x < a$ .

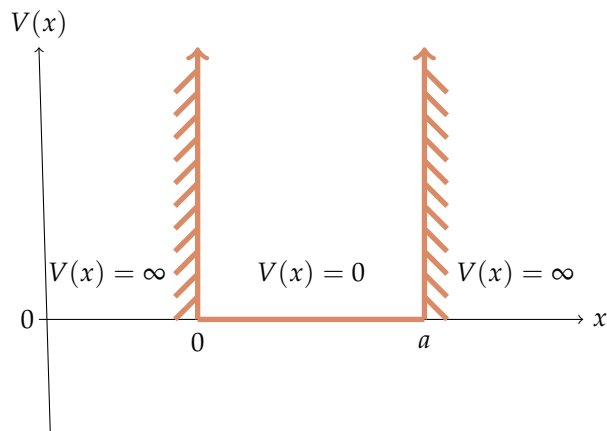


Figure 1: The potential energy of the particle is  $\infty$  outside the box, and zero inside it.

*Solution:*

The time-independent Schrödinger equation for the problem is

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x)$$

where the potential energy is

$$\begin{aligned} V &= 0; & 0 < x < a \\ &= \infty; & x < 0 \text{ or } x > a. \end{aligned}$$

The time-independent Schrödinger equation for the problem can now be written as

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) &= E\psi(x); \quad 0 < x < a \\ \Rightarrow \left[ \frac{d^2}{dx^2} + \frac{2mE}{\hbar^2} \right] \psi(x) &= 0 \\ \Rightarrow \left[ \frac{d^2}{dx^2} + \left( \frac{p}{\hbar} \right)^2 \right] \psi(x) &= 0 \end{aligned}$$

The general solution for the above equation is

$$\begin{aligned} \psi(x) &= c_1 \exp\left(ix \frac{p}{\hbar}\right) + c_2 \exp\left(-ix \frac{p}{\hbar}\right) \\ &= c_1 \left\{ \cos\left(x \frac{p}{\hbar}\right) + i \sin\left(x \frac{p}{\hbar}\right) \right\} + c_2 \left\{ \cos\left(x \frac{p}{\hbar}\right) - i \sin\left(x \frac{p}{\hbar}\right) \right\} \\ &= (c_1 + c_2) \cos\left(x \frac{p}{\hbar}\right) + i(c_1 - c_2) \sin\left(x \frac{p}{\hbar}\right) \\ &= A \cos\left(x \frac{p}{\hbar}\right) + B \sin\left(x \frac{p}{\hbar}\right) \end{aligned}$$

Now, let's us derive the same solution using another method.

*Series solution method*

Let the solution be

$$\psi(x) = \sum_{j=0}^{\infty} c_j x^j$$

The derivatives are

$$\begin{aligned} \frac{d}{dx} \psi(x) &= \sum_{j=1}^{\infty} j c_j x^{j-1} \\ &= \sum_{k=0}^{\infty} (k+1) c_{k+1} x^k \quad \text{where } k = j-1 \\ \frac{d^2}{dx^2} \psi(x) &= \sum_{j=2}^{\infty} j(j-1) c_j x^{j-2} \\ &= \sum_{k=0}^{\infty} (k+2)(k+1) c_{k+2} x^k \quad \text{where } k = j-2 \end{aligned}$$

Now the time-independent Schrödinger equation can be written as

$$\begin{aligned} \sum_{k=0}^{\infty} (k+2)(k+1) c_{k+2} x^k + \left( \frac{p}{\hbar} \right)^2 \sum_{k=0}^{\infty} c_k x^k &= 0 \\ \Rightarrow \sum_{k=0}^{\infty} \left[ (k+2)(k+1) c_{k+2} + \left( \frac{p}{\hbar} \right)^2 c_k \right] x^k &= 0 \end{aligned}$$

The above equation is true for any  $k$

$$\begin{aligned} \Rightarrow (k+2)(k+1) c_{k+2} + \left( \frac{p}{\hbar} \right)^2 c_k &= 0 \\ \Rightarrow c_{k+2} &= -\frac{1}{(k+2)(k+1)} \left( \frac{p}{\hbar} \right)^2 c_k \end{aligned}$$

$k = 0 :$

$$c_2 = -\frac{1}{2} \left(\frac{p}{\hbar}\right)^2 c_0$$

$k = 1 :$

$$c_3 = -\frac{1}{6} \left(\frac{p}{\hbar}\right)^2 c_1$$

$k = 2 :$

$$\begin{aligned} c_4 &= -\frac{1}{12} \left(\frac{p}{\hbar}\right)^2 c_2 \\ &= \frac{1}{24} \left(\frac{p}{\hbar}\right)^4 c_0 \end{aligned}$$

$k = 3 :$

$$\begin{aligned} c_5 &= -\frac{1}{20} \left(\frac{p}{\hbar}\right)^2 c_3 \\ &= \frac{1}{120} \left(\frac{p}{\hbar}\right)^5 c_1 \end{aligned}$$

$$\begin{aligned} \Rightarrow \psi(x) &= c_0 + c_1 x - \frac{1}{2} \left(\frac{p}{\hbar}\right)^2 c_0 x^2 - \frac{1}{6} \left(\frac{p}{\hbar}\right)^2 c_1 x^3 + \frac{1}{24} \left(\frac{p}{\hbar}\right)^4 c_0 x^4 + \frac{1}{120} \left(\frac{p}{\hbar}\right)^5 c_1 x^5 \dots \\ &= c_0 \left[ 1 - \frac{1}{2!} \left(\frac{p}{\hbar}\right)^2 x^2 + \frac{1}{4!} \left(\frac{p}{\hbar}\right)^4 x^4 - \dots \right] + c_1 \frac{\hbar}{p} \left[ \left(\frac{p}{\hbar}\right) x - \frac{1}{3!} \left(\frac{p}{\hbar}\right)^3 x^3 + \frac{1}{5!} \left(\frac{p}{\hbar}\right)^5 x^5 - \dots \right] \\ &= c_0 \cos\left(\frac{p}{\hbar}x\right) + c_1 \frac{\hbar}{p} \sin\left(\frac{p}{\hbar}x\right) \\ &= A \cos\left(\frac{p}{\hbar}x\right) + B \sin\left(\frac{p}{\hbar}x\right). \end{aligned}$$

We have obtained the same general solution using two different techniques. Now, we can apply the known boundary conditions for finding a particular solution.

*Introducing boundary conditions*

$$\begin{aligned} \psi(0) = 0 &\Rightarrow A \cos(0) + B \sin(0) = A = 0 \\ \psi(L) = 0 &\Rightarrow B \sin\left(\frac{p}{\hbar}L\right) = 0 \Rightarrow \frac{p}{\hbar}L = n\pi \Rightarrow \frac{p}{\hbar} = \frac{n\pi}{L} \end{aligned} \quad (1)$$

Hence the solution is

$$\psi_n(x) = B \sin\left(\frac{n\pi}{L}x\right) \quad n = 1, 2, \dots \quad (2)$$

For  $n = 0$ ,  $\psi_0(x) = 0 \forall x$  which is a trivial solution.

*Normalization*

The condition for  $\psi_n(x)$  to be normalized is

$$\int_0^\infty dx \quad \psi_n(x) = 1. \quad (3)$$

Hence

$$|B|^2 \int_0^\infty dx \sin^2\left(\frac{n\pi}{L}x\right) = 1.$$

Let us use the formula

$$\boxed{\int dx \sin^2(\alpha x) = \frac{x}{2} - \frac{\sin(2\alpha x)}{4\alpha}}$$

to get

$$\begin{aligned} |B|^2 \left[ \frac{x}{2} - \frac{\sin\left(\frac{2n\pi}{L}x\right)}{4\frac{n\pi}{L}} \right]_0^L &= 1 \\ \Rightarrow |B|^2 \frac{L}{2} &= 1 \\ \Rightarrow B &= \sqrt{\frac{2}{L}}. \end{aligned} \quad (4)$$

Hence the normalized form of the solution is given by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \quad n = 1, 2, \dots \quad (5)$$

*Energy levels*

Let us use the boundary condition Eq.(1)

$$\begin{aligned} \frac{p}{\hbar} &= \frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{L} \\ \Rightarrow E &= \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \frac{h^2 n^2}{8mL^2}. \end{aligned} \quad (6)$$


---