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

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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 $x > 0$, and $V = 0$ for $0 < x < a$.

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

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

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

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

Series solution method

Let the solution be

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

The derivatives are

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

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

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

$k = 0$:

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

$k = 1$:

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

$k = 2:$

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

$k = 3:$

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

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

Introducing boundary conditions:

$$\psi(0) = 0 \Rightarrow A\cos(0) + B\sin(0) = A = 0$$

$$\psi(L) = 0 \Rightarrow B\sin\left(\frac{p}{\hbar}L\right) = 0 \Rightarrow \frac{p}{\hbar}L = n\pi \Rightarrow \frac{p}{\hbar} = \frac{n\pi}{L} \tag{1}$$

Hence the solution is

$$\psi_n(x) = B\sin\left(\frac{n\pi}{L}x\right) \qquad n = 1, 2, \ldots. \tag{2}$$

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

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

Hence

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

Let us use the formula

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

to get

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

Hence the normalized form of the solution is given by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \qquad n = 1, 2, \ldots . \tag{5}$$

Energy levels

Let us use the boundary condition 1

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