Infinite Potential Well Problem: Expected Values of Position and Momentum

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Abstract

These are my self-study notes pertaining to the basic infinite potential well problem.

Contents

1 Infinite Potential Well - Basics

One-dimensional Schrodinger equation with time-independent potential V:

$$i\hbar\frac{\partial\Psi}{\partial t}(x,t) = -\frac{\hbar^2}{2M}\frac{\partial^2\Psi}{\partial x^2}(x,t) + V(x)\Psi(x,t) \tag{1}$$

where M stands for particle's mass.

Infinite potential well of width L is:

$$V(x) = \begin{cases} 0 & \text{if } x \in [0, L] \\ +\infty & \text{if } x \notin [0, L] \end{cases}$$

Time-independent Schrodinger equation **inside** the infinite well is:

$$-\frac{\hbar^2}{2M}\frac{d^2\psi}{dx^2}(x) = E\psi(x)$$

The n-th solution (with $n \in \mathbb{N}_+ = \{1, 2, 3, ...\}$) of the time-independent Schrodinger equation is:

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi n}{L}x\right) \tag{2}$$

Energy corresponding to the n-th solution is:

$$E_n = \frac{\hbar^2}{2M}\frac{\pi^2 n^2}{L^2} \tag{3}$$

It will be helpful to have the difference between energies for states m and n available later on:

$$E_m - E_n = \frac{\hbar^2}{2M}\frac{\pi^2}{L^2}(m^2 - n^2) \tag{4}$$

Reminder: the Hamiltionian operator $\hat{H}$ is defined to be:

$$\hat{H} := -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V$$

whereas the momentum operator is defined as:

$$\hat{p} := -i\hbar\frac{\partial}{\partial x} \tag{5}$$

Consequently, Hamiltonian can be rewritten as:

$$\hat{H} = \frac{\hat{p}^2}{2M} + V$$

Last but not least, the n-th solution of the time-independent Schrodinger equation is an eigenfunction of the Hamiltonian that corresponds to the eigenvalue E_n:

$$\hat{H}\psi_n = E_n\psi_n$$

The solution of the Schrodinger equation in the infinite well is:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \phi_n(t)\psi_n(x) \tag{6}$$

with $\phi_n(t)$ given by:

$$\phi_n(t) = \exp\left(-iE_n t/\hbar\right) \tag{7}$$

2 Partial derivative $\partial\Psi/\partial x$

Differentiating (2) with repect to position x gives:

$$\frac{\partial\Psi}{\partial x} = \sum_{n=1}^{\infty} c_n \phi_n(t) \frac{d\psi_n(x)}{dx} \tag{8}$$

Since:

$$\frac{d\psi_n}{dx} = \sqrt{\frac{2}{L}}\frac{\pi n}{L}\cos\left(\frac{\pi n}{L}x\right)$$

Then:

$$\frac{\partial\Psi}{\partial x} = \sqrt{\frac{2}{L}}\sum_{n=1}^{\infty} c_n \phi_n \frac{\pi n}{L}\cos\left(\frac{\pi n}{L}x\right) \tag{9}$$

3 Product $\Psi^*\Psi$

The wave function Ψ for IWP is:

$$\Psi = \sum_n c_n \phi_n \psi_n$$

Hence, the product $\Psi^*\Psi$ is:

$$\Psi^*\Psi = \left(\sum_m c_m^* \phi_m^* \psi_m\right)\left(\sum_n c_n^* \phi_n^* \psi_n\right) = \sum_{m,n} c_m^* c_n \phi_m^* \phi_n \psi_m \psi_n \tag{10}$$

4 Notation for Parity of Natural Numbers

Consider set of pairs of natural numbers greater than zero: $\mathbb{N}_+ \times \mathbb{N}_+$. I define the relation P, $P \subset \mathbb{N}_+ \times \mathbb{N}_+$ of identical parity of two distinct natural numbers on this set in the following manner:

$$P := \{(m, n) \in \mathbb{N}_+ \times \mathbb{N}_+ : m \neq n \wedge m \equiv n \mod 2\} \tag{11}$$

Analogously, the relation R of odd parity of pair of distinct natural numbers on this set is therefore:

$$R := \{(m, n) \in \mathbb{N}_+ \times \mathbb{N}_+ : m \neq n \wedge m \not\equiv n \mod 2\} \tag{12}$$

The sets P and R thus defined will be used later. Unsurprisingly:

$$\mathbb{N}_+ \times \mathbb{N}_+ = P \cup R \cup \{(n, n) : n \in \mathbb{N}_+\}$$

5 Useful integrals

5.1 Trigonometric identities

In this section I list the basic trigonometric identities that are needed to derive the integrals in the subsequent subsections. These are:

$$\begin{aligned}
\sin^2 x &= 1 - \cos^2 x \\
\cos^2 x &= 1 - \sin^2 x \\
\cos 2x &= \cos^2 x - \sin^2 x \\
\sin^2 x &= \frac{1}{2}(1 - \cos 2x) \\
\cos^2 x &= \frac{1}{2}(1 + \cos 2x) \\
\sin(x + y) &= \sin x \cos y + \cos x \sin y \\
\cos(x + y) &= \cos x \cos y + \sin x \sin y \\
\sin x \sin y &= \frac{1}{2}(\cos(x - y) - \cos(x + y)) \\
\sin x \cos y &= \frac{1}{2}(\sin(x + y) + \sin(x - y))
\end{aligned}$$

5.2 Integral of $\sin^2 nx$

$$I_{n,n}^{s,s} := \int \sin^2 nx dx = \frac{1}{2}\int (1-\cos 2nx)\, dx = \frac{1}{2}x - \frac{1}{4n}\sin 2nx + C$$

5.3 Integral of $\sin mx \sin nx$ for $m \neq n$

$$\begin{aligned} \int \sin mx \sin nx dx &= \frac{1}{2}\int (\cos(m-n)x - \cos(m+n)x)\, dx \\ &= \frac{\sin(m-n)x}{2(m-n)} - \frac{\sin(m+n)x}{2(m+n)} + C \end{aligned}$$

5.4 Integral of $\cos^2 nx$

$$\int \cos^2 nx dx = \frac{1}{2}\int (1+\cos 2nx)\, dx \quad = \quad \frac{1}{2}x + \frac{1}{4n}\sin 2nx + C$$

5.5 Integral of $\sin nx \cos nx$

$$\int \sin nx \cos nx dx = \frac{1}{2}\int \sin 2nx dx = -\frac{1}{4n}\cos 2nx + C$$

5.6 Integral of $\sin mx \cos nx$

$$\begin{aligned} \int \sin mx \cos nx dx &= \frac{1}{2}\int \sin(m+n)x + \sin(m-n)x dx \\ &= -\frac{1}{2(m+n)}\cos(m+n)x - \frac{1}{2(m-n)}\cos(m-n)x + C \end{aligned}$$

5.7 Integral of $x \sin^2 nx$

Integrating by parts:

$$\begin{aligned} \int x\sin^2 nx dx &= x\int \sin^2 nx dx - \int \left(\int \sin^2 nx\right) dx \\ &= \left(\frac{1}{2}x^2 - \frac{x}{4n}\sin 2nx\right) - \int \left(\frac{1}{2}x - \frac{1}{4n}\sin 2nx\right) dx \\ &= \left(\frac{1}{2}x^2 - \frac{x}{4n}\sin 2nx\right) - \left(\frac{1}{4}x^2 + \frac{1}{8n}\cos 2nx\right) + C \\ &= \frac{1}{4}x^2 - \frac{x}{4n}\sin 2nx - \frac{1}{8n}\cos 2nx + C \end{aligned}$$

5.8 Integral of $x \sin nx \sin mx$

Integration by parts yields:

$$\begin{aligned}
I &= \int x \sin mx \sin nx dx = x \int \sin mx \sin nx dx - \int \left(\int \sin mx \sin nx dx \right) dx \\
&= \left(\frac{x \sin(m-n)x}{2(m-n)} - \frac{x \sin(m+n)x}{2(m+n)} \right) \\
&\quad - \int \left(\frac{\sin(m-n)x}{2(m-n)} - \frac{\sin(m+n)x}{2(m+n)} \right) dx \\
&= \frac{x \sin(m-n)x}{2(m-n)} + \frac{x \sin(m+n)x}{2(m+n)} \\
&\quad - \left(-\frac{\cos(m-n)x}{2(m-n)^2} + \frac{\cos(m+n)x}{2(m+n)^2} \right) \\
&= \frac{x \sin(m-n)x}{2(m-n)} - \frac{x \sin(m+n)x}{2(m+n)} + \frac{\cos(m-n)x}{2(m-n)^2} - \frac{\cos(m+n)x}{2(m+n)^2} + C
\end{aligned}$$

Consequently:

$$\begin{aligned}
I &= \int x \sin mx \sin nx dx \\
&= \frac{x \sin(m-n)x}{2(m-n)} - \frac{x \sin(m+n)x}{2(m+n)} + \frac{\cos(m-n)x}{2(m-n)^2} - \frac{\cos(m+n)x}{2(m+n)^2} + C
\end{aligned}$$

6 Expected Value of an Operator

Let $\hat{A}$ be an operator representing the observable A. Then, the expected value of A is obtained from the formula:

$$\langle A \rangle = \int \Psi^* \hat{A} \Psi dx \tag{13}$$

7 Position x

The observable x is represented by operator $\hat{x} = x$ so that the expected value of position is:

$$\langle p \rangle = \int_0^L \Psi^* \hat{x} \Psi dx = \int_0^L \Psi^* x \Psi dx = \int_0^L x \Psi^* \Psi dx$$

Since:

$$\Psi = \sum_n c_n \phi_n \psi_n$$

It follows that:

$$\int_0^L x\Psi^*\Psi dx = \sum_{m,n} c_m^* c_n \phi_m^* \phi_n \int_0^L x\psi_m\psi_n dx$$

Calculating the last integral in the expression above:

$$\begin{aligned}
\int_0^L x\psi_m\psi_n dx &= \int_0^L x\frac{2}{L}\sin\frac{\pi m x}{L}\sin\frac{\pi n x}{L}dx \\
&= \frac{2}{L}\int_0^L x\sin\frac{\pi m x}{L}\sin\frac{\pi n x}{L}dx \\
&= \frac{2}{L}\int_0^\pi x\sin mx \sin nx dx
\end{aligned}$$

Let $X_{m,n}$ denote:

$$X_{m,n} = \int_0^L x\psi_m\psi_n dx \tag{14}$$

Using change of variables $x \mapsto \pi x/L$ gives:

$$X_{m,n} = \frac{2L}{\pi^2}\int_0^\pi x\sin mx \sin nx dx \tag{15}$$

7.1 $X_{m,n}$ for $m = n$

For $m = n$:

$$X_{m,n} = X_{n,n} = \frac{2L}{\pi^2}\int_0^\pi x\sin^2 nx dx \tag{16}$$

The integral in the formula for $X_{n,n}$ is readily evaluated to be:

$$\begin{aligned}
\int_0^\pi x\sin^2 nx dx &= \left[\frac{1}{4}x^2 - \frac{x}{4n}\sin 2nx - \frac{1}{8n}\cos 2nx\right]_0^\pi \\
&= \left(\frac{1}{4}\pi^2 - \frac{1}{8n}\right) - \left(0 - \frac{1}{8n}\right) = \frac{1}{4}\pi^2
\end{aligned}$$

Hence:

$$X_{n,n} = \frac{2L}{\pi^2}\frac{\pi^2}{4} = \frac{L}{2} \tag{17}$$

7.2 $X_{m,n}$ for $m \neq n$

When $m \neq n$:

$$X_{m,n} = \frac{2L}{\pi^2} \int_0^\pi x \sin mx \sin nx dx \tag{18}$$

The integral in the formula for $X_{m,n}$ is:

$$\begin{aligned}\int_0^\pi x \sin mx \sin nx dx = \bigg[&\frac{x\sin(m-n)x}{2(m-n)} - \frac{x\sin(m+n)x}{2(m+n)} \\ &+ \frac{\cos(m-n)x}{2(m-n)^2} - \frac{\cos(m+n)x}{2(m+n)^2}\bigg]_0^\pi\end{aligned}$$

Note that the values of the trigonometric functions involved in the forumula above depend on the parity of m and n. Hence, two cases need to be considered.

7.2.1 Case: m, n are of the same parity

If: $m \equiv n \mod 2$ then:

$$X_{m,n} = \frac{2L}{\pi^2} \tag{19}$$

7.2.2 Case: m, n are of different parity

If: $m \not\equiv n \mod 2$ then:

$$X_{m,n} = \frac{2L}{\pi^2}\left(\frac{-4mn}{(m+n)^2(m-n)^2}\right) = \frac{-8Lmn}{\pi^2(m-n)^2(m+n)^2} \tag{20}$$

7.3 Formula for $\langle x \rangle$

As has been demonstrated above:

$$X_{m,n} = \begin{cases} \dfrac{L}{2} & \text{if } m = n \\ 0 & \text{if } (m,n) \in P \\ \dfrac{-8Lmn}{\pi^2(m-n)^2(m+n)^2} & \text{if } (m,n) \in R \end{cases} \tag{21}$$

On substitution into formula for $\langle x \rangle$ I obtain:

$$\langle x \rangle = \sum_{(m,n)\in\mathbb{N}_+^2} c_m^* c_n \phi_m^2 \phi_n X_{m,n} \tag{22}$$

Transforming the expression further:

$$\begin{aligned}
\langle x \rangle &= \sum_{(m,n)\in\mathbb{N}_+^2} c_m^* c_n \phi_m^2 \phi_n X_{m,n} \\
&= \sum_{n=1}^{\infty} |c_n|^2 \frac{L}{2} + \sum_{(m,n)\in R} c_m^* c_n \phi_m^* \phi_n \frac{-8Lmn}{\pi^2(m-n)^2(m+n)^2}
\end{aligned}$$

So that:

$$\langle x \rangle = \frac{L}{2} - 8L \sum_{(m,n)\in R} c_m^* c_n \phi_m^* \phi_n \frac{mn}{\pi^2(m^2-n^2)^2} \tag{23}$$

8 Momentum p

Observable p is represented by opearator $\hat{p}$ equal:

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

As a result, the expected value of p is:

$$\langle p \rangle = \int \Psi^* \hat{p} \Psi dx = -i\hbar \int \Psi^* \frac{\partial \Psi}{\partial x} dx \tag{24}$$

Recall the derivative with respect to position (9):

$$\frac{\partial \Psi}{\partial x} = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} c_n \phi_n \frac{\pi n}{L} \cos\left(\frac{\pi n}{L} x\right)$$

Hence:

$$\begin{aligned}
\langle p \rangle &= -i\hbar \int \Psi^* \frac{\partial \Psi}{\partial x} dx \\
&= -i\hbar \int_0^L \left(\sum_{m=1}^{\infty} c_m^* \phi_m^* \psi_m \right) \left(\sum_{n=1}^{\infty} c_n \phi_n \frac{d\psi_n}{dx} \right) dx \\
&= -i\hbar \sum_{m,n} c_m^* c_n \phi_m^* \phi_n \int_0^L \psi_m \frac{d\psi_n}{dx} dx
\end{aligned}$$

Define:

$$Y_{m,n} := \int_0^L \psi_m \frac{d\psi_n}{dx} dx \tag{25}$$

Then, after change of variables:

$$\begin{aligned} Y_{m,n} &= \frac{2\pi n}{L^2}\int_0^L \sin\frac{\pi m}{L}x\cos\frac{\pi n}{L}xdx \\ &= \frac{2n}{L}\int_0^\pi \sin mx\cos nxdx \end{aligned}$$

8.1 $Y_{m,n}$ for $m = n$

$$\begin{aligned} Y_{n,n} &= \frac{n}{L}\int_0^L 2\sin nx\cos nxdx && (26)\\ &= \frac{n}{L}\int_0^L \sin 2nxdx = \frac{n}{L}\left[-\frac{1}{2n}\cos 2nx\right]_0^\pi && (27)\\ &= \frac{1}{2L}\left((-1)-(-1)\right) = 0 && (28) \end{aligned}$$

8.2 $Y_{m,n}$ for $m \neq n$

When $m \neq n$:

$$\begin{aligned} Y_{m,n} &= \frac{2n}{L}\int_0^\pi \sin mx\cos nxdx \\ &= \frac{2n}{L}\left[-\frac{1}{2(m+n)}\cos(m+n)x - \frac{1}{2(m-n)}\cos(m-n)x\right]_0^\pi \end{aligned}$$

8.2.1 Case: m, n are of the same parity

$$Y_{m,n} = \frac{2n}{L}\left[\left(-\frac{1}{2(m+n)} - \frac{1}{2(m-n)}\right) - \left(-\frac{1}{2(m+n)} - \frac{1}{2(m-n)}\right)\right] = 0$$

8.2.2 Case: m, n are of different parities

$$\begin{aligned} Y_{m,n} &= \frac{2n}{L}\left[\left(\frac{1}{2(m+n)} + \frac{1}{2(m-n)}\right) - \left(-\frac{1}{2(m+n)} - \frac{1}{2(m-n)}\right)\right] \\ &= \frac{4mn}{L(m^2-n^2)} \end{aligned}$$

8.3 Formula for $\langle p \rangle$

It has been demonstrated above that:

$$Y_{m,n} = \begin{cases} 0 & \text{if } m = n \text{ or } (m,n) \in P \\ \dfrac{-8Lmn}{\pi^2(m-n)^2(m+n)^2} & \text{if } (m,n) \in R \end{cases} \tag{29}$$

Substituting the values of $Y_{m,n}$ into the formula for $\langle p \rangle$ yields:

$$\begin{aligned} \langle p \rangle &= -i\hbar \sum_{m,n} c_m^* c_n \phi_m^* \phi_n Y_{m,n} \\ &= -\frac{4i\hbar}{L} \sum_{(m,n)\in R} c_m^* c_n \phi_m^* \phi_n \frac{mn}{m^2 - n^2} \end{aligned}$$

9 Ehrenfest's Theorem - Check for IWP's Position and Momentum

According to Erhenfest's theorem for position and momentum the following equality holds:

$$M \frac{d\langle x \rangle}{dt} = \langle p \rangle \tag{30}$$

By (23) the derivative $d\langle x \rangle / dt$ is:

$$\frac{d\langle x \rangle}{dt} = -8L \sum_{(m,n)\in P'} c_m^* c_n \frac{mn}{\pi^2(m^2-n^2)^2} \frac{d(\phi_m^* \phi_n)}{dt} \tag{31}$$

The time derivative of the product $\phi_m \phi_n$ is needed:

$$\begin{aligned} \frac{d(\phi_m^* \phi_n)}{dt} &= \frac{d}{dt} \exp\left(\frac{it}{\hbar}(E_m - E_n)\right) \\ &= \frac{d}{dt} \exp\left(\frac{it}{\hbar} \frac{\hbar^2 \pi^2 (m^2 - n^2)}{2ML^2}\right) \\ &= \frac{d}{dt} \exp\left(it \frac{\hbar \pi^2}{2ML^2}(m^2 - n^2)\right) \\ &= i \frac{\hbar \pi^2}{2ML^2}(m^2 - n^2) \phi_m^* \phi_n \end{aligned}$$

Substituting into the formula for $d\langle x\rangle/dt$:

$$\frac{d\langle x\rangle}{dt} = -\frac{4i\hbar}{ML} \sum_{(m,n)\in P'} c_m^* c_n \phi_m \phi_n \frac{mn}{m^2 - n^2} \tag{32}$$

So we see that the equality (30) holds.