Infinite Potential Well: Various Considerations

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Abstract

This notebook contains various facts and considerations related to one-dimensional Schrodinger equation for infinite well potential.

Contents

1 Infinite Potential Well - Basics

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

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

Infinite potential well of width L is:

$$V(x) = \begin{cases} 0 & \text{if } x \in [0,L] \\ +\infty & \text{if } x \notin [0,L] \end{cases} \tag{2}$$

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

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}(x) = E\psi(x) \tag{3}$$

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

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n}{L} x\right) \tag{4}$$

Energy corresponding to the n-th solution is:

$$E_n = \frac{\hbar^2}{2m} \frac{\pi^2 n^2}{L^2} \tag{5}$$

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

$$\hat{H} := -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \tag{6}$$

whereas the momentum operator is defined as:

$$\hat{p} := -i\hbar \frac{\partial}{\partial x} \tag{7}$$

Consequently, Hamiltonian can be rewritten as:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V \tag{8}$$

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:

$$\hat{H}\psi_n = E_n \psi_n \tag{9}$$

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

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \phi_n(t) \psi_n(x) \tag{10}$$

with $\phi_n(t)$ given by:

$$\phi_n(t) = \exp\{-iE_n t/\hbar\} \tag{11}$$

2 Expected Value of Momentum in Ifinite Well

I am considering the following expectation:

$$< p >= \int_0^L \Psi^* \hat{p} \Psi dx \tag{12}$$

Substituting (10) I obtain:

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

I am working out the following integral I_{mn} now:

$$I_{mn} := \int_0^L \psi_m(x)\frac{d\psi_n(x)}{dx} dx \tag{13}$$

The derivative $d\psi_n/dx$ is:

$$\frac{d\psi_n(x)}{dx} = \sqrt{\frac{2}{L}}\frac{\pi n}{L}\cos\left(\frac{\pi n}{L}x\right) \tag{14}$$

Therefore:

$$I_{mn} = \frac{2\pi n}{L^2}\int_0^L \sin\left(\frac{\pi n}{L}x\right)\cos\left(\frac{\pi n}{L}x\right) dx \tag{15}$$

After change of variables $x \mapsto (\pi n/L)x$ the integral I_{mn} becomes:

$$I_{mn} = \frac{2n}{L}\int_0^{\pi} \sin mx \cos nx dx \tag{16}$$

Let T_{mn} be:

$$T_{mn} := \int_0^{\pi} \sin mx \cos nx dx \tag{17}$$

It can be shown that T_{mn} (cf. appendix A) is:

$$T_{mn} = \begin{cases} 0 & \text{if } m = n \text{ or if } m \equiv n \mod 2 \\ \frac{m}{m^2 - n^2} & \text{if } m \not\equiv n \mod 2 \end{cases} \tag{18}$$

Consequently, I_{mn} is non zero only when $m \neq n$ and $m \not\equiv n \mod 2$, when it equals:

$$I_{mn} = \frac{2mnL}{m^2 - n^2} \tag{19}$$

3 Matrix Representation of the Momentum Operator $\hat{p}$ in Infinite Potential Well

Let $P = [p_{ij}]$ be the matrix representing the momentum operator. The element p_{ij} of the matrix P is given by:

$$p_{ij} = \int_0^L \Psi_i^* \hat{p} \Psi_j dx \tag{20}$$

Operator $\hat{p}$ applied to Ψ_j is:

$$\hat{p}\Psi_j = -i\hbar \frac{\partial \Psi_j}{\partial x} = \tag{21}$$

Appendix A Integral T_{mn}

In order to calculate the integral T_{mn}:

$$T_{mn} := \int_0^\pi \sin mx \cos nx dx \tag{22}$$

it is necessary to get rid of the product of sine and cosine function of different arguments.

Let's consider, however, the case $m = n$ first. It is easy to show that if $m = n$, then $T_{mn} = T_{nn} = 0$.

Back to the case $m \neq n$ It can be shown[1] that:

$$\sin mx \cos nx = \frac{1}{2} \left(\sin\left((m+n)x\right) + \sin\left((m-n)x\right) \right) \tag{23}$$

Hence, the integral T_{mn} can be rewritten as:

$$T_{mn} = \frac{1}{2} \int_0^\pi \sin\left((m+n)x\right) dx + \frac{1}{2} \int_0^\pi \sin\left((m-n)x\right) dx \tag{24}$$

When we calculate this integral, we see that the final value of T_{mn} depends on whether m and n are of the same parity or not. The final result obtained after a little bit of simple algebra is:

$$T_{mn} = \begin{cases} 0 & \text{if } m = n \text{ or if } m \equiv n \mod 2 \\ \frac{m}{m^2 - n^2} & \text{if } m \not\equiv n \mod 2 \end{cases} \tag{25}$$

[1] To derive this use the high school formula $\sin(x + y) = \sin x \cos y + \cos x \sin y$ and its flavor with $-y$ substituted for y.