QUANTUM MECHANICS: LECTURE 7

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Abstract

This lecture analyses the particle in 1-D box problem.

CONTENTS

DESCRIPTION OF THE PROBLEM

We discuss here an application to the mathematical axioms of quantum mechanics studied earlier to a simple, yet important problem. The quantum particle in an infinite potential well, or a particle in a box see figure 1. This is

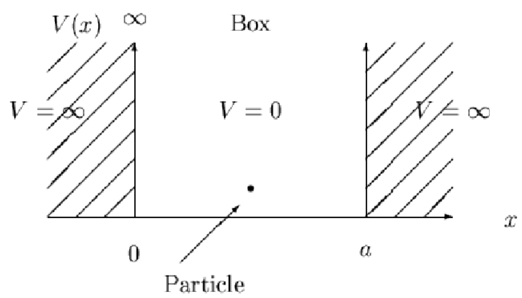

Figure 1: A diagram illustrating the particle in a box problem

an idealisation for a large enough potential compared to the particle's energy. This problem is very important example to study discrete spectrum .
We start by a particle trapped in a potential well, of width a. The Schrödinger's equation for this particle is written as - in position representation-:

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

With :

$$V(x) = \begin{cases} 0, & \text{for } 0 < x < a \\ \infty, & \text{otherwise} \end{cases} \tag{2}$$

Since the above equation is clearly separable, similar to the free particle. It resembles a stationary state. We then write the eigenvalue problem:

$$\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}u(x;E) + V(x)u(x;E) = Eu(x;E) \tag{3}$$

The energy eigenfunctions are then equal to $\psi(x,t;E) = u(x;E)\; e^{-i\hbar\omega t}$

We now attempt to solve (3) subject to the boundary conditions:

$$u(x=0) = u(x=a) = 0 \tag{4}$$

Because there is a null probability of the particle being outside the box. And the second condition on the wavefunction :

$$\frac{du(x)}{dx}|_{x=0} = \frac{du(x)}{dx}|_{x=a} \tag{5}$$

This condition comes from naturally from the analysis of the problem. The first derivative of the wavefunction is proportional to the momentum of the particle, we expect the particle will 'bump' with both walls in the same manner. Although, this violates the *Born conditions* discussed in lecture 5, but keep in mind that the infinite well is an unphysical example!
Now, we rewrite Schrödinger's equation as:

$$\frac{d^2u(x)}{dx^2} + k^2u(x) = 0 \tag{6}$$

with $k = \sqrt{2mE}\hbar$; this differential equation is solved by the substitution $u(x) = e^{Rx}$ Resulting:

$$u(x) = Ae^{ikx} + Be^{-ikx} \tag{7}$$

Where A and B are constants, we use the identity :

We observe that, using the boundary conditions we obtain :

$$ik\left(Ae^{ika} - Be^{-ika}\right) = ik(A-B)$$

$$\Rightarrow u(x) = C\sin(kx) \tag{8}$$

$$u(a) = C\sin(ka) = 0$$

$$\Rightarrow k = \frac{n\pi}{a} \tag{9}$$

But since $k = \sqrt{2mE}\hbar$, we conclude that energy takes discrete values :

$$\begin{aligned} E_n =& \frac{\hbar^2 n^2 \pi^2}{2ma^2} \\ =& E_0\, n^2 \end{aligned} \tag{10}$$

With $E_0 = \frac{\hbar^2\pi^2}{2ma^2}$, the ground energy. And n here denotes the **quantum number** for the excited states of the particle in the box. Now, we may write the energy-eigenfunctions, after calculating the normalisation factor $C = \sqrt{\frac{2}{a}}e^{i\varphi}$:

we add always an arbitrary phase factor $e^{i\varphi}$

$$\psi_n(x,t) = \sqrt{\frac{2}{a}}\left(\sin(\frac{n\pi x}{a})\right)e^{i(\omega t+\phi)} \tag{11}$$

The total wavefunction is written as, by the superposition principle :

$$\psi(x,t) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty}\left(\sin(\frac{n\pi x}{a})\right)e^{i(\omega t+\phi)} \tag{12}$$

Which is a Fourier series (we could have obtained this solution immediately by Fourier analysis). The following figure demonstrates the eigenfunctions for various excitation states, and the probability density function ρ:

MOMENTUM EIGENFUCNTIONS

We now turn into calculation the Fourier transform of $u(x)$ in order to compute the momentum eigenfucntions $\phi(p,t)$:

$$v(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_0^a dx\, \underbrace{e^{\frac{i}{\hbar}px}}_{\langle p|x\rangle}\underbrace{u(x)}_{\langle x|u\rangle} \tag{13}$$

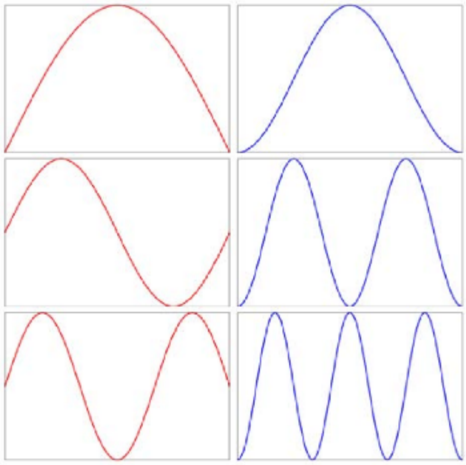

Figure 2: First,second, and third lowest-energy eigenfunctions (red) and associated probability densities (blue) for the infinite square well potential

substituting with $u(x)$ we have:

$$v(p) = \frac{1}{\sqrt{\pi a \hbar}} \int_0^a dx \, e^{\frac{i}{\hbar}px} \, \sin(n\hbar px) \tag{14}$$

Evaluation of this integral gives:

The following identity was used : $\int e^{ax} \sin bx \, dx = \frac{e^{ax}}{a^2+b^2} (a \sin bx + b \cos bx)$

$$v(p) = n\sqrt{\frac{a\pi}{\hbar}} \left(\frac{1-(-1)^n \, e^{-\frac{i}{\hbar}pa}}{n^2\pi^2 - a^2\frac{p^2}{\hbar^2}} \right) \tag{15}$$

Plotting the momentum probability density function - for various excitations - : This calculation ends the basic analysis for a particle in a box, what remains

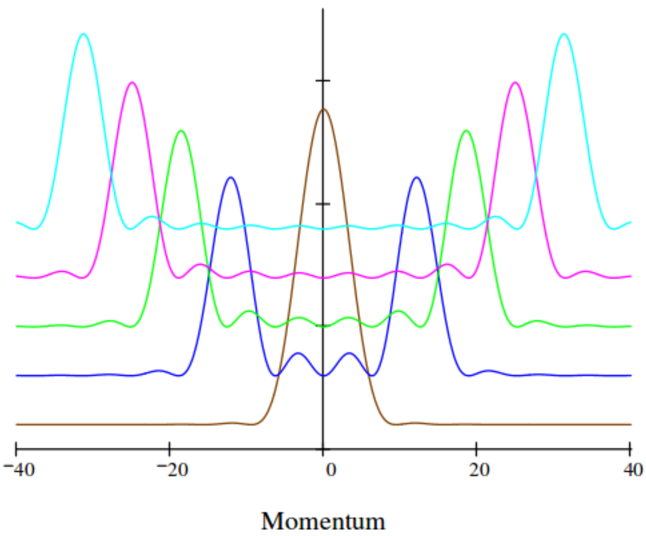

Figure 3: Momentum probability density function for the ground state and three more excitation states.

is the calculation of the expected values for some dynamical observables, which is left for tutorials.

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