PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 13, March 11, 2021 (Thursday)

- Reading: Time-Independent Schrödinger Equation [Griffiths 2]
- Assignment: Problem Set 6 due March 12 (Friday).
  Submit your homework assignments to Canvas.
- Midterm Exam on March 16 (Tuesday) 1:00 pm–3:00 pm

Topics for Today: Schrödinger Equation [Chapter 2 in Griffiths]

3.6 Schrödinger Equation

(a) Infinite Square Well [Griffiths 2.2]

(b) Free Particle [Griffiths 2.4]

(c) The Delta-Function Potential [Griffiths 2.5]

Topics for Next Lecture: Schrödinger Equation [Chapter 2 in Griffiths]

(d) Finite Square Well [Griffiths 2.6]

3.7 Stationary State Solutions

3.8 Equation of continuity

3.6 The Schrödinger Equation

(a) Infinite square well potential

Let us consider the potential

$$V(x) = \begin{cases} 0 & \text{for } x^2 < a^2, \text{ and} \\ \infty, & \text{for } x^2 \geq a^2. \end{cases}$$

To examine the motion of a particle in this potential, let us attempt to solve the equation of motion (EOM) for

$$V(x) = \begin{cases} 0, & \text{for } x^2 < a^2, \text{ i.e. } -a < x < a \\ V_0, & \text{for } x^2 \geq a^2, \text{ i.e. } x \leq -a \text{ or } x \geq a. \end{cases}$$

with $a > 0$ and take the limit $V_0 \to \infty$.

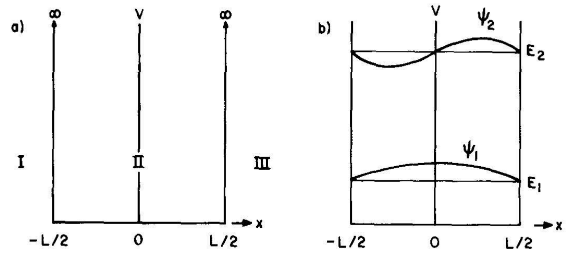

Figure 1: The infinite square well potential with $a =$ L/2.

In the $x-$basis the Hamiltonian is given by

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

and the Schrödinger equation is

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

The potential is different in different regions. Thus we consider Region (I): $x \leq -a$, Region (II): $-a < x < a$, and Region (III): $x \geq a$.

Region (I): $x \leq -a$, with $V_0 > E > 0$, the EOM is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_0\psi(x) = E\psi(x) \quad \text{or} \quad \frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi(x) = 0\,.$$

Hence

$$\psi(x) = A_1 e^{-\lambda x} + B_1 e^{\lambda x} \quad \text{with} \quad \lambda = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

where A_1 and B_1 are constants. If the wave function has to retain a probabilistic interpretation for a physical solution, A_1 must vanish. Otherwise, it grows exponentially with distance and would not converge. Thus for $x < -a$,

$$\psi(x) = B_1 e^{\lambda x}.$$

However, $\lambda \to \infty$ as $V_0 \to \infty$. Therefore, in this limit

$$\psi(x) = 0, \;\; \text{for} \;\; x \leq -a.$$

Similarly, in Region (III): for $x \geq a$, with $V_0 > E > 0$, the EOM is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_0\psi(x) = E\psi(x) \quad \text{or} \quad \frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi(x) = 0\,.$$

Hence

$$\psi(x) = A_3 e^{-\lambda x} + B_3 e^{\lambda x} \quad \text{with} \quad \lambda = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

where A_3 and B_3 are constants. If the wave function has to retain a probabilistic interpretation for a physical solution, B_3 must vanish. Otherwise, it grows exponentially with distance and would not converge. Thus for $x > a$,

$$\psi(x) = A_3 e^{-\lambda x}\,.$$

However, $\lambda \to \infty$ as $V_0 \to \infty$. Therefore, in this limit

$$\psi(x) = 0, \;\; \text{for} \;\; x \geq a.$$

Region (II): $-a < x < a$, the equation of motion (EOM) is

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

or

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x)\,.$$

In the standard form, the equation of motion becomes

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

where

$$k^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad k = \sqrt{\frac{2mE}{\hbar^2}}\,.$$

Find the characteristic equation an the general solution.

The EOM is a linear second order homogeneous differential equation. The characteristic equation is

$$\lambda^2 + k^2 = 0$$

with roots

$$\lambda_{1,2} = \pm ik \quad \text{with} \quad k = \sqrt{\frac{2mE}{\hbar^2}}\,.$$

Hence the general solution is

$$\psi(x) = Ae^{\lambda_1 x} + Be^{\lambda_2 x} = Ae^{+ikx} + Be^{-ikx}$$

or

$$\psi(x) \quad = \quad C\sin(kx) + D\cos(kx)$$

where C and D are constants.

The solution has to be continuous everywhere and in particular at the boundary. Thus matching solutions at $x = \pm a$, we have

$$\begin{aligned} \psi(a) &= C\sin(ka) + D\cos(ka) \;=\; 0 \quad \text{and} \\ \psi(-a) &= -C\sin(ka) + D\cos(ka) \;=\; 0\,. \end{aligned}$$

There are two nontrivial solutions.

(a) Even function solution with $C = 0$ and $\cos(ka) = 0$,

$$\begin{aligned} k_n(2a) &= n\pi\,, \quad k_n \;=\; \frac{n\pi}{2a}\,, \quad k_n^2 \;=\; \frac{n^2\pi^2}{4a^2}\,, \quad n = 1, 3, 5, \cdots \\ E_n &= \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{8ma^2} \end{aligned}$$

where n is an odd integer and $\cos(k_n x)$ is an even function. Thus

$$\begin{aligned} \Psi(x,t) &= \sum D_n \psi_n(x) e^{-(i/\hbar)E_n t}\,, \quad \text{where} \\ \psi_n(x) &= \frac{1}{\sqrt{a}}\cos(k_n x)\,, \quad n = 1, 3, 5, \cdots\,. \end{aligned}$$

(b) Odd function solution with $D = 0$ and $\sin(ka) = 0$,

$$\begin{aligned} k_n(2a) &= n\pi\,, \quad n = 2, 4, 6, \cdots \\ k_n &= \frac{n\pi}{2a} \\ k_n^2 &= \frac{n^2\pi^2}{4a^2} \\ E_n &= \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{8ma^2}\,. \end{aligned}$$

where n is an even integer and $\sin(k_n x)$ is an odd function. Thus

$$\Psi(x,t) = \sum C_n \psi_n(x) e^{-(i/\hbar)E_n t}$$

where

$$\psi_n(x) = \frac{1}{\sqrt{a}} \sin(k_n x)\,, \quad n = 2, 4, 6, \cdots\,.$$

In summary, we have eigen-functions of the Hamiltonian for the infinite square well

$$\psi_n(x) = \frac{1}{\sqrt{a}} \cos(k_n x) = \frac{1}{\sqrt{a}} \cos\left(\frac{n\pi x}{2a}\right) , \quad n = 1, 3, 5, \cdots$$

and

$$\psi_n(x) = \frac{1}{\sqrt{a}} \sin(k_n x) = \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi x}{2a}\right) , \quad n = 2, 4, 6, \cdots$$

with

$$k_n = \frac{n\pi}{2a} \quad \text{and} \quad E_n = \frac{p^2}{2m} = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{8ma^2} .$$

The ground state and the first excited state have the energy

$$\begin{aligned} E_1 &= \frac{\hbar^2 \pi^2}{8ma^2} , \quad n = 1 , \quad \text{and} \\ E_2 &= \frac{\hbar^2 \pi^2}{2ma^2} , \quad n = 2 . \end{aligned}$$

Orthogonal Functions

Here are useful identities for orthonormal functions.

(i)

$$\begin{aligned}\int_{-a}^{a} \sin^2\left(\frac{\pi x}{a}\right) dx &= \left(\frac{a}{\pi}\right)\int_{-\pi}^{\pi} \sin^2 u \, du \\ &= \left(\frac{a}{\pi}\right)\left[\frac{u}{2} - \frac{\sin^2 u}{4}\right]\Bigg|_{u=-\pi}^{\pi} = a\end{aligned}$$

where we have applied

$$u = \frac{\pi x}{a}\,, \quad du = \frac{\pi}{a} dx\,, \quad \text{and} \quad u = \pm\pi \quad \text{for} \quad x = \pm a\,.$$

(ii)

$$\int_{-a}^{a} \sin\left(\frac{\pi x}{a}\right)\cos\left(\frac{3\pi x}{2a}\right) dx = 0 \quad \text{odd integrand}\,.$$

Useful integrals

$$\int \cos^2(x)dx = \frac{x}{2} + \frac{\sin 2x}{4}\,,$$
$$\int \sin^2(x)dx = \frac{x}{2} - \frac{\sin 2x}{4}\,,$$

and

$$\int_{-a}^{a} \cos(k_m x)\cos(k_n x)dx = 0 \quad \text{for} \quad m \neq n\,,$$
$$\int_{-a}^{a} \sin(k_m x)\sin(k_n x)dx = 0 \quad \text{for} \quad m \neq n\,,$$
$$\int_{-a}^{a} \cos(k_m x)\sin(k_n x)dx = 0 \quad \text{(odd function)}$$

where

$$k_n = \frac{n\pi}{2a} \qquad m, n \in N\,.$$

One of the things we notice immediately is that whereas classically for any $E > 0$ particle is allowed, quantum mechanically particle motion is allowed only for discrete values of the energy.
Energy for this system is quantized.

We also see that for this system

$$\psi(x) = 0 \quad \text{for } |x| \geq a$$

and

$$\lim_{|x|\to\infty} \psi(x) = 0\,.$$

Such a system is called a bound state.

Such a system is called a bound state and for every bound state we have quantization of energy. A very familiar example is the Hydrogen atom. Furthermore, in the present system

$$\psi(x) = 0 \ \text{ for } \ x^2 \geq a^2$$

This system is equivalent to a particle inside a box of length $2a$.

Exercise

Normalize the solutions. Calculate ΔX for the ground state. Estimate the ground state energy from the uncertainty principle and compare it with the actual value.

Exercise

Plot the first few solutions and describe their qualitative features. In particular show that the nth state has $n-1$ nodes inside the well.

(b) Free particle in one dimension

In general, the Schrödinger Equation is

$$i\hbar\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle \quad \text{with} \quad H = \frac{P^2}{2m} + V(X)\,.$$

For a free particle the potential energy is zero: $V(X) = 0$.

In the $p-$basis the Schrödinger equation becomes

$$i\hbar\frac{d}{dt}\langle p|\Psi\rangle = \langle p|H|\Psi\rangle = \frac{p^2}{2m}\langle p|\Psi\rangle\,,$$

where we have applied the eigenvalue equation

$$P|p\rangle = p|p\rangle\,, \quad \frac{P^2}{2m}|p\rangle = \frac{p^2}{2m}|p\rangle\,, \quad \text{and} \qquad \langle p|\frac{P^2}{2m} = \langle p|\frac{p^2}{2m}\,.$$

Defining the wave function in the momentum space as

$$\phi(p) \equiv \langle p|\Psi\rangle$$

we obtain

$$i\hbar \frac{d\phi(p)}{dt} = \frac{p^2}{2m}\phi(p)\,.$$

Homework:

(a) Show that the general solution of this differential equation is

$$\phi(p) = N e^{-\frac{i}{\hbar}\left(\frac{p^2}{2m}\right)t}$$

where N is the normalization constant.

(b) Apply inverse Fourier transform and find the wave function $\psi(x)$ in the coordinate space.

In the $x-$basis, the Schrödinger Equation becomes

$$\begin{aligned} i\hbar\frac{d}{dt}\langle x|\Psi(t)\rangle &= \int \langle x|\frac{P^2}{2m}|y\rangle\langle y|\Psi(t)\rangle\, dy \\ i\hbar\frac{\partial}{\partial t}\Psi(x,t) &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x,t) \quad \text{or} \quad \frac{\partial}{\partial t}\Psi(x,t) = \frac{i\hbar}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) \end{aligned}$$

This is like a heat equation except that the coefficient is imaginary. This solution can be written as

$$\Psi(x,t) = \frac{N}{(a^2 + i\hbar t/m)^{1/2}} e^{-x^2/2(a^2+i\hbar t/m)}$$

where "a" is a constant which can be determined from the value of the initial wave function. The constant N is determined from normalization of the probability. The probability density is given by

$$\psi^*\psi = \frac{N^2}{a(a^2 + \hbar^2 t^2/m^2 a^2)^{1/2}} e^{-x^2/(a^2+\hbar^2 t^2/m^2 a^2)}\,.$$

Thus we see that a free particle is denoted by a Gaussian. Furthermore, the probability of finding a particle peaks around $x = 0$ and has a mean width of

$$\frac{1}{2}(a^2 + \frac{\hbar^2 t^2}{m^2 a^2})$$

Thus we see that by choosing an appropriate constant 'a' we can localize the particle initially but as time grows the width of the Gaussian increases. This is known as the dispersion of the wave packet.

Homework

Derive the same result by working in the momentum basis and then transforming to the $x-$basis.

(c) The Delta-Function Potential [Griffiths 2.5]

Homework:

Let us consider a particle bound in a delta function potential in one dimension

$$V(x) = -\alpha\delta(x), \;\; \alpha > 0,$$

where α is a constant and the total energy $E < 0$.

Let us consider Region I for $x < 0$ and Region III for $x > 0$.

In Region I and Region III, the Schrödinger equation is

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

where $E < 0$ for a bound state. The general solution of this equation is

$$\psi_i(x) = A_i e^{-kx} + B_i e^{+kx} \quad \text{for} \quad i = 1, 3\,.$$

In Region II, that is the region near $x = 0$ with $-\epsilon < x < \epsilon$, we have

$$\lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) - \alpha \delta(x) \psi(x) \right] dx \quad = \quad \lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} E \psi(x)\, dx \ \ \text{or}$$

$$\lim_{\epsilon \to 0} -\frac{\hbar^2}{2m} \left[\psi_3'(\epsilon) - \psi_1'(-\epsilon) \right] - \alpha \psi(0) \quad = \quad 0\,.$$

Then we have

$$\psi_1'(x = 0) - \psi_3'(x = 0) = \frac{2m\alpha}{\hbar^2} \psi(0) \quad \text{where} \quad \psi'(x) = \frac{d\psi}{dx}$$

has a finite jump (discontinuity) at $x = 0$ while $\psi(x)$ is continuous at $x = 0$ with

$$B_1 = A_3 = A\,.$$

Let us choose A to be real and find the normalized continuous wave function. For all x, i.e., $-\infty \leq x \leq \infty$, we have

$$\psi(x) = A e^{-k|x|}\,.$$