PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 12, March 09, 2021 (Tuesday)

- Handout: Solutions to Problem Set 5.
- Reading: Time-Independent Schrödinger Equation [Griffiths 2]
- Assignment: Problem Set 6 due March 12 (Friday).
  Submit your homework assignments to Canvas.

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

3.6 Schrödinger Equation

(a) Infinite Square Well [Griffiths 2.2]

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

(a) Infinite Square Well [Griffiths 2.2]

(b) Free Particle [Griffiths 2.4]

(c) Finite Square Well [Griffiths 2.6]

(d) Potential of a Barrier (Bonus)

3.7 Stationary State Solutions

3.8 Equation of continuity

3.6 The Schrödinger Equation

The Schrödinger equation is

$$H|\Psi(t)\rangle = E|\Psi(t)\rangle \ \text{ i.e. } \ H|\Psi(t)\rangle = i\hbar\frac{d}{dt}|\Psi(t)\rangle \ \text{ or } \ i\hbar\frac{d|\Psi(t)\rangle}{dt} = H|\Psi(t)\rangle\,.$$

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

$$i\hbar\frac{d}{dt}\langle x|\Psi(t)\rangle = \int\langle x|H|y\rangle\langle y|\Psi(t)\rangle dy$$

where the wave function is $\Psi(x,t) \equiv \langle x|\Psi(t)\rangle$, and the matrix elements of X, $V(X)$, P, P^2, and H become

- $\langle x|X|y\rangle$ and $\langle x|V(X)|y\rangle$
- $\langle x|P|y\rangle$ and $\langle x|P^2|y\rangle$
- $\langle x|H|y\rangle$

The Schrödinger equation is

$$i\hbar \frac{d|\Psi(t)\rangle}{dt} = H|\Psi(t)\rangle \, .$$

In the $x-$basis, the relevant matrix elements become

- $\langle x|X|y\rangle = y\delta(x-y)$ and $\langle x|V(X)|y\rangle = V(y)\delta(x-y)$,
- $$\langle x|P|y\rangle = -i\hbar \frac{\partial}{\partial x}\delta(x-y) \quad \text{and} \quad \langle x|P^2|y\rangle = -\hbar^2 \frac{\partial^2}{\partial x^2}\delta(x-y) \, ,$$

and

$$\langle x|H|y\rangle = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(y)\right]\delta(x-y) \, .$$

And the Schrödinger equation becomes

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t) \, .$$

Introducing separation of variables $\Psi(x,t) = f(t)u(x)$, we obtain

$$\begin{aligned} i\hbar\left(\frac{df}{dt}\right)u(x) &= f(t)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]u(x) \\ i\hbar\frac{df/dt}{f} &= \frac{1}{u}\left[-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + V(x)u(x)\right] = E\,. \end{aligned}$$

Since the left-hand side depends only on time and the right-hand side depends only on spatial coordinates, both sides must be equal to a constant which we call E. Thus

$$\begin{aligned} i\hbar\frac{df}{dt} &= Ef \quad \text{with} \quad f(t) = A_t e^{-(\frac{i}{\hbar})Et} \\ \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]u(x) &= Eu(x)\,. \end{aligned}$$

In the energy basis

$$\Psi(x,t) = u(x)f(t) = u(x)e^{-(\frac{i}{\hbar})Et} = \psi(x)e^{-(\frac{i}{\hbar})Et}$$

where we have absorbed the normalization constant A_t into $u(x)$.

If the Hamiltonian does not depend on time explicitly, we have the time independent Schrödinger equation

$$H\psi_n(x) = E_n\psi_n(x) \quad \text{eigenvalue equation}$$

where E_n are eigenvalues of the Hamiltonian operator H.

The general solution to the equation of motion becomes

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n\psi_n(x)e^{-(\frac{i}{\hbar})E_n t} = \sum_{n=0}^{\infty} c_n\Psi_n(x,t)\,.$$

The separable solutions

$$\Psi_n(x,t) = \psi_n(x)e^{-(\frac{i}{\hbar})E_n t}$$

are stationary states, such that probabilities and expectation values are independent of time.

(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 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 $V_0 \to \infty$.

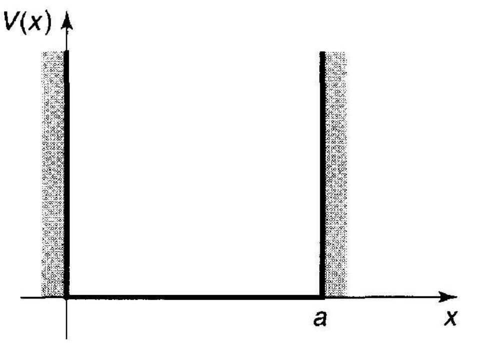

Figure 1: The infinite square well potential.

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): $x \le -a$, Region (II): $-a < x < a$, and Region (III): $x \ge a$.

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

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

where C and D are constants.