Lecture 4

Michael Brodskiy
Professor: G. Fiete

February 19, 2025

- Wave Equation for Unidimensional Particle
  - In classical mechanics, we have the energy problem, with E as the total energy, T as the kinetic energy, and V as the potential energy:

$$E = T + V = \frac{p^2}{2m} + V(x)$$

  - In quantum mechanics, we may define the Hamiltonian as:

$$\hat{H} = \frac{\hat{p}}{2m} + V(\hat{x})$$

    * Where $\hat{p}$ is the momentum operator and $\hat{x}$ is the position
  - From here, the time-independent Schrödinger equation may be written as:

$$\hat{H}\phi_E(x) = E\phi_E(x)$$

    * Where $\phi_E(x)$ represents the wave function/eigenfunction
  - We may continue to get:

$$\hat{p} = -i\hbar\frac{d}{dx}, \quad \hat{x} = x$$

    * This can be used to obtain:

$$\hat{p}\phi(x) = -i\hbar\frac{d}{dx}\phi(x), \quad \hat{x}\phi(x) = x\phi(x)$$

  - From here, we get:

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

- The above is the wave equation we need to solve. The wave function can generically be written as:

$$\psi(x) = \sum_{n=0}^{d} \psi_n \phi_{E_n}(x)$$

  * Note that ψ_n is a scalar coefficient (projections of ψ along the n-th direction) and $\phi_{E_n}(x)$ represents basis functions
  * Also, note that, from previous lessons, we may recall that the probability of finding the system in a particular eigenstate is:

$$P_{E_n} = |\psi_n|^2$$

- In Dirac notation:

$$|\psi\rangle = \begin{pmatrix} \langle E_1|\psi\rangle \\ \langle E_2|\psi\rangle \\ \vdots \\ \langle E_n|\psi\rangle \end{pmatrix}$$

  * And also:

$$\langle\psi| = \begin{pmatrix} \langle E_1|\psi\rangle^* & \langle E_2|\psi\rangle^* & \cdots & \langle E_n|\psi\rangle^* \end{pmatrix}$$

- Change of Basis
  * Changing basis to a position representation allows us to obtain the probability of finding the particle at x as:

$$P_x = |\psi(x)|^2$$

  * This means that $|\psi(x)|^2$ is now a probability density such that:

$$\int_{-\infty}^{\infty} P(x)\, dx = \int_{-\infty}^{\infty} |\psi(x)|^2\, dx = 1$$

  * Furthermore, we may find the probability that the particle is in a certain range as:

$$P[a \leq x \leq b] = \int_a^b P(x)\, dx = \int_a^b |\psi(x)|^2\, dx$$

  * In summary, we determine:

$$\langle x|\psi\rangle = \psi(x)$$
$$\langle\psi|x\rangle = \psi^*(x)$$
$$\hat{A} = \hat{A}(x)$$