Review of Quantum Mechanics I (part 2)

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Free Particle

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where} \quad k = \frac{\sqrt{2mE}}{\hbar}. \tag{1}$$

The general solution of the time-independent Schrödinger equation is

$$\psi(x) = Ae^{ikx} + Be^{-ikx}. \tag{2}$$

Then, taking on the time dependence, $e^{-iET/\hbar}$,

$$\Psi(x,t) = Ae^{ik(x-\frac{\hbar k}{2m}t)} + Be^{-ik(x+\frac{\hbar k}{2m}t)}. \tag{3}$$

- Traveling waves (not stationary).
- Not normalizable.

Free Particle

We introduce a wave packet as an initial wave function,

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk. \tag{4}$$

Fourier and Inverse Fourier Transform

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk \iff \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(k) e^{-ikx} dx$$

Then the general separable solution of the free particle is

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(x) e^{i(kx - \frac{\hbar k^2}{2m} t)} dk, \tag{5}$$

with

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx. \tag{6}$$

Infinite Potential Well

When a particle is in a infinite potential well with

$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases} \tag{7}$$

- outside: $\psi(x) = 0$
- inside: $\psi(x)$ obeys the time-independent Schrödinger equation with $V = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi,$$

or

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where} \quad k = \frac{\sqrt{2mE}}{\hbar}. \tag{8}$$

General Solution and Boundary Conditions

The general solutions is

$$\psi(x) = A \sin kx + B \cos kx. \tag{9}$$

Then, boundary conditions are

$$\psi(0) = \psi(a) = 0 \tag{10}$$

because ψ and the derivative of ψ must be continuous.

Applying the condition $\psi(0) = 0$, we obtain $B = 0$, and hence

$$\psi(x) = A \sin kx. \tag{11}$$

General Solution and Boundary Conditions

Applying the condition $\psi(a) = 0$ to $\psi(x) = A \sin kx$, we obtain the quantization of energy

$$ka = \pm n\pi, \quad \text{with} \quad n = 0, 1, 2, \cdots, \tag{12}$$

where $k = 0$ is a trivial solution ($\psi(x) = 0$). Then,

$$k_n = \frac{n\pi}{a}, \quad \text{with} \quad n = 1, 2, 3, \cdots \tag{13}$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}. \tag{14}$$

And, the wave functions are

$$\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right). \tag{15}$$

Revisited: Infinite Potential Well

- Symmetry
- The larger the number of nodes, the higher the energy.
- Orthogonality

$$\int \psi_m(x)^* \psi_n(x) dx = \delta_{mn}.$$

- Completeness

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x),$$

$$c_n = \int \psi_n(x)^* f(x) dx.$$

Where to go next...

We need to go back to some mathematics,
linear algebra and vector spaces.