POSTECH 이성익 교수의
양자 세계에 관한 강연
- 3장 -

편집 도우미: **POSTECH** 학부생 정윤영

Chapter 3

Eigenvalues, Eigenfunctions, and the Expansion Postulate

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

Time dependent Schrödinger equation

$\psi(x,t)=T(t)\cdot u(x)$,

$$i\hbar u(x)\frac{dT(t)}{dt}=-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}T(t)+V(x)\cdot T(t)\cdot u(x)$$

$$\therefore\frac{i\hbar\dfrac{dT(t)}{dt}}{T(t)}=-\frac{\hbar^2}{2m}\frac{\dfrac{d^2u(x)}{dx^2}}{u(x)}+V(x)=E$$

E is a constant.

$$i\hbar\frac{dT(t)}{dt}=E\cdot T(t)$$

$$\therefore T(t)=A\cdot e^{\frac{E}{i\hbar}t}=A\cdot e^{-iwt}$$

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

Time independent Schrödinger equation

$$H\cdot\psi=E\cdot\psi\ ,\qquad H=-\frac{\hbar^2}{2m}\nabla^2+V$$

E:Eigenvalue Ψ:Eigenfunction

Free particle에서 E<0,

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

$$\frac{d^2u(x)}{dx^2}=-\frac{2mE}{\hbar^2}\cdot u(x)=\kappa^2\cdot u(x)$$

$$\therefore u(x)=Ae^{-\kappa x}+Be^{\kappa x}=0$$

$$(\because probability=1)$$

→ E<0인 particle은 존재하지 않는다.

Free particle에서 E>0,

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

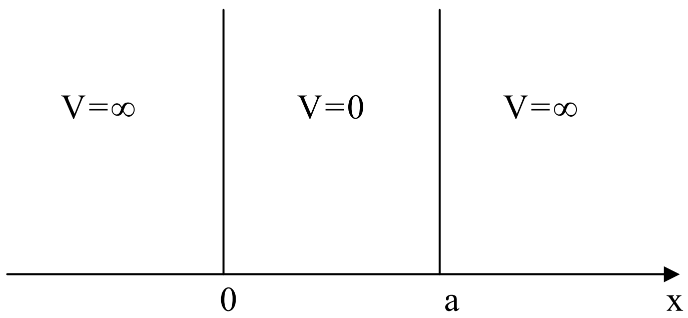
$$\frac{d^2u(x)}{dx^2}=-\frac{2mE}{\hbar^2}\cdot u(x)=-k^2\cdot u(x) \qquad k=\frac{\sqrt{2mE}}{\hbar}$$

$$(\because E>0)$$

$$\therefore u(x)=A\sin kx+B\cos kx=A'e^{ikx}+B'e^{-ikx}$$

$$\therefore \psi(x,t)=A''e^{i(kx-wt)}+B''e^{i(-kx-wt)}$$

1-D infinite potential well



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

$x \le 0$ & $x \ge a$,

$$\psi(x) = 0$$

$0 \le x \le a$,

$\psi(x) = A\sin kx + B\cos kx$ 이 때의 energy는 $E = \dfrac{\hbar^2 k^2}{2m}$

$$\psi(0) = \psi(a) = 0$$

$$\therefore \psi(x) = A\sin\frac{n\pi}{a}x$$

$$E_n = \left(\frac{\hbar^2\pi^2}{2ma^2}\right)n^2 \qquad k_n = \frac{n\pi}{a} \qquad n = 1, 2, 3, 4, \cdots$$

→ energy is quantized

자연이 극도로 싫어하는 Infinite potential에 대한 문제이기 때문에 boundary에서 $\dfrac{d\psi(x)}{dx}$가 연속이 아니다.

Schrödinger equation은 linear equation이다.

$\therefore \psi = a_1\psi_1 + a_2\psi_2 + a_3\psi_3 + \cdots = \sum_{m=1}^{\infty} a_m\psi_m$ 도 해가 된다.

$$\psi_1 = \sqrt{\frac{2}{a}}\sin\frac{\pi}{a}x$$

$$1 = \int_{-\infty}^{\infty} \psi_1^* \psi_1 dx \qquad 0 = \int_{-\infty}^{\infty} \psi_1\psi_2 dx$$

$$\therefore \int_{-\infty}^{\infty} \psi_m\psi_n dx = \delta_{m,n}$$

$$\psi = \sum_{m=1}^{\infty} a_m \psi_m \qquad \psi_m \otimes \psi_n = \delta_{m,n}$$

$\psi_1, \psi_2, \psi_3, \cdots$은 서로 linearly independent하다.

$$\psi(x) = \sum_{n=1}^{\infty} A_n \cdot u_n(x) \leftarrow \text{vector space} \quad (u_1, u_2, u_3, \cdots, u_\infty)$$

$$\int_0^a u_m^*(x) \cdot u_n(x)\, dx = \delta_{m,n}$$

$$A_m = \int_0^a u_m^*(x) \cdot \psi(x)\, dx$$

Ψ가 위와 같은 vector space로 표현 가능하면 "complete set"이다.

$$H \cdot u_n(x) = E_n \cdot u_n(x)$$

$$\langle H \rangle = \int_0^\infty \psi^*(x) \cdot H \cdot \psi(x)\, dx = \int_0^\infty \psi^*(x) \cdot H \cdot \left(\sum_{n=1}^{\infty} A_n \cdot u_n(x) \right) dx$$

$$= \sum_{n=1}^{\infty} A_n \int_0^\infty \psi^*(x) \cdot H \cdot u_n(x)\, dx = \sum_{n=1}^{\infty} A_n \int_0^\infty \psi^*(x) \cdot E_n \cdot u_n(x)\, dx$$

$$= \sum_{n=1}^{\infty} A_n \cdot E_n \int_0^\infty \psi^*(x) u_n(x)\, dx = \sum_{n=1}^{\infty} A_n \cdot E_n \cdot A_n^*$$

$$\therefore \langle H \rangle = \sum_{n=1}^{\infty} |A_n|^2 \cdot E_n \qquad 1 = \sum_{n=1}^{\infty} |A_n|^2$$

Parity Operator

$\psi(x)=\psi(-x)$: even parity

$\psi(x)=-\psi(-x)$: odd parity

$$\underline{P}\psi(x)=\psi(-x)$$
$$\underline{P}\psi^{+}(x)=\psi(x)$$
$$\underline{P}\psi^{-}(x)=-\psi^{-}(x)$$

+: even parity
-: odd parity

Parity operator의 eigenvalue는 ±1

$$\underline{P}u(x)=\lambda u(x)$$
$$\underline{P}^2u(x)=u(x)=\underline{P}\,\underline{P}u(x)=\underline{P}\lambda u(x)=\lambda^2u(x)$$
$$\therefore \lambda=\pm1$$

If $H(x)=H(-x)$, $PH=HP$

$$\therefore [H,P]=0$$

→ Hamiltonian operator와 parity operator가 commute 한다.

두 operator가 commute하면, 두 operator를 동시에 만족시키는 simultaneous eigenfunction이 존재할 수 있다.

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

만약 potential이 even function이면,

$$H(x)=H(-x)$$
$$\therefore [H,P]=0$$