POSTECH 이성익 교수의
양자 세계에 관한 강연
- 5장 -

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Chapter 5

The General Structure of Wave Mechanics

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t)$$

$$H \cdot u_E(x) = E \cdot u_E(x)$$

$$H = \frac{P_{op}^2}{2m} + V(x) = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + V(x)$$

Requirement $\int \psi^* \psi \, dx < \infty$

$$\psi(x) = \sum_E C_E u_E(x)$$ ← Complete Set

$$\int u_{E'}^*(x) u_{E''}(x) dx = \delta_{E'E''}$$: Orthogonality

∴ Coefficient를 계산할 수 있다.

$$\int u_{E'}^*(x)\psi(x)dx = \int u_{E'}^*(x) \sum_E C_E u_E(x) dx = C_{E'}$$

Spectrum of eigenvalue

$$\psi(x) = \underbrace{\sum_n C_n u_{E_n}(x)}_{\text{Bounded solution}} + \underbrace{\int C(E) u_E(x) dE}_{\text{Continuous solution}}$$

$$\int u_{E_m}^*(x) \cdot u_{E_n}(x) dx = \delta_{m,n}$$

$$\int u_E^*(x) \cdot u_{E'}(x) dx = \delta(E - E')$$

Hermitian Conjugate operator

$$+:\quad \int \left[A\cdot\psi(x)\right]^{*}\cdot\psi(x)dx \equiv \int \psi^{*}(x)\cdot A^{+}\cdot\psi(x)dx$$

Time dependence and Classical limit

$$\langle A\rangle_t = \int \psi^{*}(x,t)\cdot A\cdot\psi(x,t)\,dx$$

$$\frac{d\langle A\rangle_t}{dt} = \int \psi^{*}(x,t)\cdot\frac{\partial A}{\partial t}\cdot\psi(x,t)\,dx$$

$$+\int \frac{\partial\psi^{*}(x,t)}{\partial t}\cdot A\cdot\psi(x,t)\,dx + \int\psi^{*}(x,t)\cdot A\cdot\frac{\partial\psi(x,t)}{\partial t}dx$$

$$= \int \psi^{*}(x,t)\cdot\frac{\partial A}{\partial t}\cdot\psi(x,t)\,dx$$

$$+\int \frac{H\cdot\psi^{*}(x,t)}{-i\hbar}\cdot A\cdot\psi(x,t)\,dx + \int\psi^{*}(x,t)\cdot A\cdot\frac{H\cdot\psi(x,t)}{i\hbar}dx$$

$$= \left\langle\frac{\partial A}{\partial t}\right\rangle + \frac{1}{i\hbar}\int\psi^{*}(x,t)\cdot A\cdot H\cdot\psi(x,t) - H\cdot\psi^{*}(x,t)\cdot A\cdot\psi(x,t)\,dx$$

$$\left(\begin{aligned} &H\cdot\psi^{*}(x,t)\cdot A\cdot\psi(x,t) = \left[H^{+}\cdot\psi(x,t)\right]^{*}\cdot A\cdot\psi(x,t) \\ &= \psi(x,t)^{*}\cdot H\cdot A\cdot\psi(x,t) \end{aligned}\right)$$

$$= \left\langle\frac{\partial A}{\partial t}\right\rangle + \frac{1}{i\hbar}\int\psi^{*}(x,t)\cdot[A,H]\cdot\psi(x,t)\,dx$$

$$= \left\langle\frac{\partial A}{\partial t}\right\rangle + \frac{i}{\hbar}\langle[H,A]\rangle$$

$$\therefore\ \frac{d\langle A\rangle_t}{dt} = \left\langle\frac{\partial A}{\partial t}\right\rangle_t + \frac{i}{\hbar}\langle[H,A]\rangle_t$$

If $\frac{\partial A}{\partial t}=0$ and $[H,A]=0$, $\frac{d\langle A\rangle_t}{dt}=0$.

$\therefore$potential이 time-invariant이면, 입자의 energy는 보존된다.
(Hamiltonian의 expectation value=energy)

$$\frac{d\langle p\rangle_t}{dt}=\left\langle\frac{\partial p}{\partial t}\right\rangle_t+\frac{i}{\hbar}\langle[H,p]\rangle_t=0+\frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m}+V(x),p\right]\right\rangle_t$$

$$=\frac{i}{\hbar}\langle[V(x),p]\rangle_t$$

$\therefore$potential이 constant이면, 입자의 momentum은 보존된다.

$$\frac{d\langle x\rangle_t}{dt}=\frac{\langle p\rangle_t}{m}$$

$$\frac{d\langle x\rangle_t}{dt}=\left\langle\frac{\partial x}{\partial t}\right\rangle_t+\frac{i}{\hbar}\langle[H,x]\rangle_t=0+\frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m}+V(x),x\right]\right\rangle_t$$

$$=\frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m},x\right]\right\rangle_t=\frac{i}{2m\hbar}\left\langle\left[p^2,x\right]\right\rangle_t$$

$$\left(\begin{aligned}&\left[p^2,x\right]=-2i\hbar p\\&[A\cdot B,C]=A\cdot B\cdot C-C\cdot A\cdot B\\&\qquad=A\cdot B\cdot C-A\cdot C\cdot B+A\cdot C\cdot B-C\cdot A\cdot B\\&\qquad=A\cdot[B,C]+[A,C]\cdot B\end{aligned}\right)$$

$$=\frac{i}{2m\hbar}\langle -2i\hbar p\rangle_t=\frac{\langle p\rangle_t}{m}$$

$$\frac{d\langle p\rangle_t}{dt} = -\left\langle \frac{dV}{dx} \right\rangle_t$$

$$\frac{d\langle p\rangle_t}{dt} = \left\langle \frac{\partial p}{\partial t} \right\rangle_t + \frac{i}{\hbar}\langle [H, p] \rangle_t = 0 + \frac{i}{\hbar}\left\langle \left[\frac{p^2}{2m} + V(x), p \right] \right\rangle_t$$

$$\left(p_{op} = \frac{\hbar}{i} \cdot \frac{\partial}{\partial x} \right)$$

$$= \frac{i}{\hbar}\langle [V(x), p] \rangle_t = \frac{i}{\hbar}\langle V(x) \cdot p - p \cdot V(x) \rangle_t$$

$$= \left\langle V(x) \cdot \frac{i}{\hbar} p - \frac{i}{\hbar} p \cdot V(x) \right\rangle_t$$

$$= \left\langle V(x) \cdot \frac{\partial}{\partial x} - \frac{\partial V(x)}{\partial x} \right\rangle_t$$

$$= -\left\langle \frac{\partial V(x)}{\partial x} \right\rangle_t$$