POSTECH 이성익 교수의
양자 세계에 관한 강연
- 2장 -

편집 도우미: POSTECH 학부생 정윤영

Chapter 2

Wave Particle Duality, Probability, and the Schrödinger Equation

$$\psi(x,t)=\int_{-\infty}^{\infty} A(k)e^{i(kx-wt)}dk$$

t=0에서,

$$\psi(x)=\int_{-\infty}^{\infty} g(k)e^{ikx}dk$$

이때 $g(k)=e^{-\alpha(k-k_0)^2}$ 로 주어지면

$$\psi(x)=\int_{-\infty}^{\infty} e^{-\alpha(k-k_0)^2}\cdot e^{ikx}dk=\int_{-\infty}^{\infty} e^{-\alpha\left(k^2-2k_0k+k_0{}^2-\frac{ikx}{\alpha}\right)}dk$$

$$-\alpha\left(k^2-2k_0k+k_0{}^2-\frac{ikx}{\alpha}\right)=-\alpha\left(k^2-2\left(k_0+\frac{ix}{2\alpha}\right)k+k_0{}^2\right)$$

$$=-\alpha\left(k^2-2\left(k_0+\frac{ix}{2\alpha}\right)k+k_0{}^2\right)$$

$$=-\alpha\left(k^2-2\left(k_0+\frac{ix}{2\alpha}\right)k+\left(k_0+\frac{ix}{2\alpha}\right)^2+k_0{}^2-k_0{}^2-\frac{ik_0x}{\alpha}+\frac{x^2}{4\alpha^2}\right)$$

$$=-\alpha\left(\left(k-k_0-\frac{ix}{2\alpha}\right)^2+\frac{x^2}{4\alpha^2}-\frac{ik_0x}{\alpha}\right)$$

$$\psi(x)=\sqrt{\frac{\pi}{\alpha}}\cdot e^{-\alpha\left(\frac{x^2}{4\alpha^2}-\frac{ik_0x}{\alpha}\right)}=\sqrt{\frac{\pi}{\alpha}}\cdot e^{ik_0x}\cdot e^{-\frac{x^2}{4\alpha}}$$

Free space에 있는 wave는 시간이 지남에 따라 퍼져나갈 것이다.

$$\psi(x,t)=\int_{-\infty}^{\infty}A(k)e^{ik(x-vt)}dk = f(x-vt)$$

$$\left(e^{ikx-iwt}=e^{i\frac{2\pi}{\lambda}x-i2\pi vt}=e^{2\pi i\left(\frac{x}{\lambda}-vt\right)}=e^{2\pi i\left(\frac{x}{\lambda}-\frac{v}{\lambda}t\right)}=e^{ik(x-vt)} \right)$$

$$\psi(x,t)=\int_{-\infty}^{\infty}A(k)e^{i(kx-w(k)t)}dk$$

$A(k)=e^{-\alpha(k-k_0)^2}$ 로 주어지면,

$$\psi(x,t)=\int_{-\infty}^{\infty}e^{-\alpha(k-k_0)^2}e^{i(kx-w(k)t)}dk$$

$$w(k)\cong w(k_0)+(k-k_0)\left(\frac{dw}{dk}\right)_{k=k_0}+\frac{1}{2}(k-k_0)^2\left(\frac{d^2w}{dk^2}\right)_{k=k_0}$$

$$=w(k_0)+v_g\,(k-k_0)+\beta\,(k-k_0)^2 \qquad\qquad k-k_0=k^{'}$$

$$\psi(x,t)=\int_{-\infty}^{\infty}e^{-\alpha(k-k_0)^2}e^{ikx}e^{-iw(k)t}dk=\int_{-\infty}^{\infty}e^{-\alpha k^{'2}}e^{ik^{'}x}e^{ik_0x}e^{-iw(k_0)t}e^{-iv_gk^{'}t}e^{-i\beta k^{'2}t}dk^{'}$$

$$=\int_{-\infty}^{\infty}e^{-\alpha k^{'2}}e^{ik^{'}x}e^{-i\left(v_gk^{'}+\beta k^{'2}\right)t}e^{ik_0x}e^{-iw(k_0)t}dk^{'}$$

$$=e^{ik_0x}e^{-iw(k_0)t}\int_{-\infty}^{\infty}e^{-\alpha k^{'2}}e^{-i\beta tk^{'2}}e^{ik^{'}(x-v_gt)}dk^{'}$$

$$=e^{i(k_0x-w(k_0)t)}\int_{-\infty}^{\infty}e^{ik^{'}(x-v_gt)}e^{-(\alpha+i\beta t)k^{'2}}dk^{'}$$

$$=e^{i(k_0x-w(k_0)t)}\int_{-\infty}^{\infty}e^{-(\alpha+i\beta t)\left(k^{'2}-\frac{ik^{'}(x-v_gt)}{\alpha+i\beta t}\right)}dk^{'}$$

$$=e^{i(k_0x-w(k_0)t)}\int_{-\infty}^{\infty}e^{-(\alpha+i\beta t)\left(k^{'}-\frac{i(x-v_gt)}{2(\alpha+i\beta t)}\right)^2-\frac{(x-v_gt)^2}{4(\alpha+i\beta t)}}dk^{'}$$

$$= e^{i(k_0 x - w(k_0)t)} e^{-\frac{(x-v_g t)^2}{4(\alpha+i\beta t)}} \int_{-\infty}^{\infty} e^{-(\alpha+i\beta t)\left(k' - \frac{i(x-v_g t)}{2(\alpha+i\beta t)}\right)^2} dk'$$

$$= e^{i(k_0 x - w(k_0)t)} \left(\frac{\pi}{\alpha+i\beta t}\right)^{\frac{1}{2}} e^{-\frac{(x-v_g t)^2}{4(\alpha+i\beta t)}}$$

$$\psi^*(x,t) = e^{-i(k_0 x - w(k_0)t)} \left(\frac{\pi}{\alpha-i\beta t}\right)^{\frac{1}{2}} e^{-\frac{(x-v_g t)^2}{4(\alpha-i\beta t)}}$$

$$|\psi(x,t)|^2 = \left(\frac{\pi^2}{\alpha^2+\beta^2 t^2}\right)^{\frac{1}{2}} \cdot e^{-\frac{\alpha(x-v_g t)^2}{2(\alpha^2+\beta^2 t^2)}}$$

Schrödinger Equation

free space에서,

$$p = \frac{h}{\lambda} = h\frac{k}{2\pi} = \hbar k \qquad E = h\nu = \frac{h}{2\pi}2\pi\nu = \hbar w$$

$$\psi(x,t) = \int_{-\infty}^{\infty} A(k) e^{i(kx-wt)} dk = \int_{-\infty}^{\infty} \phi(p) e^{i(px-Et)/\hbar} dp$$

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \int_{-\infty}^{\infty} \phi(p)\left(-\frac{iE}{h}\right)(i\hbar) e^{i(px-Et)/\hbar} dp = E\int_{-\infty}^{\infty} \phi(p) e^{i(px-Et)/\hbar} dp$$

$$= E\psi(x,t) = \frac{p^2}{2m}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}$$

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

→ given by nature

Potential이 있으면,

$$E = \frac{p^2}{2m} + V$$

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

Max Born,

$$|\psi|^2 = \psi^* \cdot \psi \rightarrow probability$$

$$P(x,t)\,dx = |\psi(x,t)|^2\,dx$$

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

Uncertainty Principle

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

이 것을 Bohr의 수소 원자모형에 응용하면,

$$r \cdot p \sim \hbar$$

$$E = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r} \simeq \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$\frac{\partial E}{\partial r} = -\frac{\hbar^2}{mr^3} + \frac{e^2}{4\pi\varepsilon_0 r^2} = 0$$

$$\frac{\hbar^2}{mr} = \frac{e^2}{4\pi\varepsilon_0}$$

$$r = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = \frac{\hbar}{mc}\frac{4\pi\varepsilon_0\hbar c}{e^2} = \frac{\hbar}{mc}\frac{1}{\alpha}$$

$$E \simeq \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\varepsilon_0 r} = \frac{\hbar^2}{2m}\frac{m^2c^2\alpha^2}{\hbar^2} - \frac{e^2}{4\pi\varepsilon_0}\frac{mc\alpha}{\hbar}$$

$$= \frac{mc^2}{2}\alpha^2 - mc^2\alpha^2 = -\frac{mc^2}{2}\alpha^2$$

Conjugate Equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \qquad \frac{\partial\psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{i\hbar}V\psi$$

$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2} + V\psi^* \qquad \frac{\partial\psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial x^2} - \frac{1}{i\hbar}V\psi^*$$

$$\frac{\partial}{\partial t}P(x,t) = \frac{\partial}{\partial t}\left(\psi^*(x,t)\cdot\psi(x,t)\right)$$

$$= \frac{\partial\psi^*(x,t)}{\partial t}\psi(x,t) + \frac{\partial\psi(x,t)}{\partial t}\psi^*(x,t)$$

$$= -\frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial x^2}\psi - \frac{1}{i\hbar}V\psi^*\psi + \frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2}\psi^* + \frac{1}{i\hbar}V\psi\psi^*$$

$$= -\frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial x^2}\psi + \frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2}\psi^* = \frac{i\hbar}{2m}\left(\psi^*\frac{\partial^2\psi}{\partial x^2} - \psi\frac{\partial^2\psi^*}{\partial x^2}\right)$$

$$= \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)$$

$\frac{\partial P}{\partial t} + \nabla\cdot\vec{j} = 0$ -> continuity equation

$$j = \frac{-i\hbar}{2m}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)$$

$$\left\langle f(x) \right\rangle = \int_{-\infty}^{\infty} f(x) P(x,t)\, dx = \int_{-\infty}^{\infty} \psi^*(x,t)\, f(x) \psi(x,t)\, dx$$

$$\left\langle p \right\rangle = m \frac{d\left\langle x \right\rangle}{dt}$$

$$= m \frac{d}{dt} \int_{-\infty}^{\infty} \psi^*(x,t)\, x\psi(x,t)\, dx = m \int_{-\infty}^{\infty} \left(\frac{d\psi^*}{dt} x\psi + \frac{d\psi}{dt} x\psi^* \right) dx$$

$$= m \int_{-\infty}^{\infty} \left(\left(-\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} - \frac{1}{i\hbar} V\psi^* \right) x\psi + \left(\frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{i\hbar} V\psi \right) x\psi^* \right) dx$$

$$= m \int_{-\infty}^{\infty} \left(-\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} x\psi - \frac{1}{i\hbar} V\psi^* x\psi + \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} x\psi^* + \frac{1}{i\hbar} V\psi x\psi^* \right) dx$$

$$= m \int_{-\infty}^{\infty} \left(-\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} x\psi + \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} x\psi^* \right) dx$$

$$= m \int_{-\infty}^{\infty} \frac{\hbar}{2mi} \left(\frac{\partial^2 \psi^*}{\partial x^2} x\psi - \frac{\partial^2 \psi}{\partial x^2} x\psi^* \right) dx$$

$$= \frac{\hbar}{2i} \int_{-\infty}^{\infty} \left(\frac{\partial^2 \psi^*}{\partial x^2} x\psi - \frac{\partial^2 \psi}{\partial x^2} x\psi^* \right) dx$$

$$\frac{\partial^2 \psi^*}{\partial x^2} x\psi - \frac{\partial^2 \psi}{\partial x^2} x\psi^*$$

$$= \frac{\partial}{\partial x} \left(\frac{\partial \psi^*}{\partial x} x\psi - \frac{\partial \psi}{\partial x} x\psi^* \right) - \frac{\partial \psi^*}{\partial x} \left(\psi + x \frac{\partial \psi}{\partial x} \right) + \frac{\partial \psi}{\partial x} \left(\psi^* + x \frac{\partial \psi^*}{\partial x} \right)$$

$$= \frac{\partial}{\partial x} \left(\frac{\partial \psi^*}{\partial x} x\psi - \frac{\partial \psi}{\partial x} x\psi^* \right) - \frac{\partial \psi^*}{\partial x} \psi + \frac{\partial \psi}{\partial x} \psi^*$$

$$= \frac{\hbar}{2i} \int_{-\infty}^{\infty} \left(\frac{\partial}{\partial x} \left(\frac{\partial \psi^*}{\partial x} x\psi - \frac{\partial \psi}{\partial x} x\psi^* \right) + \frac{\partial \psi}{\partial x} \psi^* - \psi \frac{\partial \psi^*}{\partial x} \right) dx$$

$$= \frac{\hbar}{2i} \int_{-\infty}^{\infty} \left(-\frac{\partial \psi^*}{\partial x} \psi + \psi^* \frac{\partial \psi}{\partial x} \right) dx = \frac{\hbar}{2i} \int_{-\infty}^{\infty} \left(\psi^* \frac{\partial \psi}{\partial x} + \psi^* \frac{\partial \psi}{\partial x} \right) dx$$

$$=\frac{\hbar}{i}\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}dx=\int_{-\infty}^{\infty}\psi^*\frac{\hbar}{i}\frac{\partial}{\partial x}\psi dx$$

$$\therefore\langle p\rangle=\int_{-\infty}^{\infty}\psi^*(x,t)\cdot\frac{\hbar}{i}\frac{\partial}{\partial x}\cdot\psi(x,t)dx \qquad p=\frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$\langle f(p)\rangle=\int_{-\infty}^{\infty}\psi^*(x,t)\cdot f\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\cdot\psi(x,t)dx$$

t=0 일 때,

$$\psi(x)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\phi(p)e^{ipx/\hbar}dp$$

$$=\sqrt{\frac{\hbar}{2\pi}}\int_{-\infty}^{\infty}\phi(\hbar k)e^{ikx}dk$$

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

$$\phi(p)=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x)e^{-ipx/\hbar}dx$$

$$\int_{-\infty}^{\infty}\phi^*(p)\cdot\phi(p)dp=\int_{-\infty}^{\infty}\phi^*(p)\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x)e^{-ipx/\hbar}dx\right)dp$$

$$=\int_{-\infty}^{\infty}\psi(x)\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\phi^*(p)e^{-ipx/\hbar}dp\right)dx$$

$$=\int_{-\infty}^{\infty}\psi(x)\cdot\psi^*(x)dx=1$$

$$\therefore \int_{-\infty}^{\infty} \phi^*(p)\cdot\phi(p)\,dp = 1$$

$$\langle p\rangle = \int_{-\infty}^{\infty} \psi^*(x)\cdot\frac{\hbar}{i}\frac{\partial}{\partial x}\cdot\psi(x)\,dx$$

$$= \int_{-\infty}^{\infty} \psi^*(x)\cdot\frac{\hbar}{i}\frac{\partial}{\partial x}\cdot\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\phi(p)e^{ipx/\hbar}dp\right)dx$$

$$= \int_{-\infty}^{\infty} \psi^*(x)\cdot\frac{\hbar}{i}\frac{ip}{\hbar}\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\phi(p)e^{ipx/\hbar}dp\right)dx$$

$$= \int_{-\infty}^{\infty} \phi(p)\cdot p\cdot\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi^*(x)e^{ipx/\hbar}dx\right)dp$$

$$= \int_{-\infty}^{\infty} \phi(p)\cdot p\cdot\phi^*(p)\,dp$$

$$\therefore \langle p\rangle = \int_{-\infty}^{\infty} \phi^*(p)\cdot p\cdot\phi(p)\,dp$$

$$\langle f(x)\rangle = \int_{-\infty}^{\infty} \phi^*(p)\cdot f\left(i\hbar\frac{\partial}{\partial p}\right)\cdot\phi(p)\,dp \qquad x = i\hbar\frac{\partial}{\partial p}$$

Generally, operators do not commute

$$[A, B] = AB - BA$$

$$[p, x]\psi(x) = \left[\frac{\hbar}{i}\frac{\partial}{\partial x}, x\right]\psi(x)$$

$$= \left(\frac{\hbar}{i}\frac{\partial}{\partial x}x - x\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi(x)$$

$$= \frac{\hbar}{i}\frac{\partial}{\partial x}x\psi(x) - x\frac{\hbar}{i}\frac{\partial\psi(x)}{\partial x}$$

$$= \frac{\hbar}{i}\psi(x) + x\frac{\hbar}{i}\frac{\partial\psi(x)}{\partial x} - x\frac{\hbar}{i}\frac{\partial\psi(x)}{\partial x}$$

$$= -i\hbar\psi(x)$$

$$\therefore [p, x] = -i\hbar$$

$$\langle p\rangle - \langle p\rangle^* = \int_{-\infty}^{\infty}\psi^*(x)\cdot\frac{\hbar}{i}\frac{\partial}{\partial x}\cdot\psi(x)\,dx - \int_{-\infty}^{\infty}\psi(x)\cdot\left(-\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\cdot\psi^*(x)\,dx$$

$$= \frac{\hbar}{i}\int_{-\infty}^{\infty}\psi^*(x)\cdot\frac{\partial}{\partial x}\psi(x) + \psi(x)\cdot\frac{\partial}{\partial x}\psi^*(x)\,dx$$

$$= \frac{\hbar}{i}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left(\psi^*(x)\cdot\psi(x)\right)dx = \frac{\hbar}{i}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}|\psi(x)|^2\,dx$$

$$= \frac{\hbar}{i}\left(|\psi(x)|^2\Big|_{x=\infty} - |\psi(x)|^2\Big|_{x=-\infty}\right)$$

$$= 0$$