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8 Valne funkcije i vektori stanja

8.1 Čestica je u kvantnom stanju opisanom valnom funkcijom

$$\Psi(x) = \begin{cases} \dfrac{1}{\sqrt{2L}}, & |x| \le L \\ 0, & |x| > L \end{cases}$$

(a) Kolika je gustoća vjerojatnosti $\rho(p)$ nalaženja čestice s impulsom p?
(b) Nacrtajte gustoću vjerojatnosti $\rho(p)$ i diskutirajte povezanost s relacijom neodređenosti.
(c) Neka je ρ_1 gustoća vjerojatnosti nalaženja čestice s impulsom $h/(4L)$. Pokažite da je

$$\frac{\rho_1}{\rho(p=0)} = \frac{4}{\pi^2}$$

8.2 Nađite valnu funkciju iz impulsnog prostora $\Phi_n(p, t)$ za n-to stacionarno stanje za problem beskonačne, pravokutne potencijalne jame širine a. Konstruirajte $|\Phi_n|^2$. Pokažite da je $|\Phi_n|^2$ konačan za $p = \pm n\pi\hbar/a$.

8.3 Izračunajte matrični element $\langle x'|H|\alpha\rangle$ gdje je $|\alpha\rangle$ po volji odabran ket, a H hamiltonijan

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

Kako će se rezultat promijeniti ako je $|\alpha\rangle$ svojstveni vektor od H?

8.4 Napišite vremenski neovisnu Schrödingerovu jednadžbu u p-reprezentaciji.

8.5 Pokažite da je svojstvena funkcija operatora položaja x jednaka delta funkciji $\delta(x - x')$, a odgovarajuća svojstvena vrijednost x'.

8.6 Pokažite da vrijedi

$$\langle p'|x|\alpha\rangle = -\frac{\hbar}{i}\frac{\partial}{\partial p'}\langle p'|\alpha\rangle$$

$\boxed{8.1}$

(a) Tražimo valnu funkciju iz impulsnog prostora

$$\langle p|\psi\rangle = \psi(p) = \int_{-L}^{L} dx \langle p|x\rangle \underbrace{\langle x|\psi\rangle}_{\frac{1}{\sqrt{2L}}} = \frac{1}{\sqrt{2L}} \int_{-L}^{L} dx \langle p|x\rangle$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}$$

$$\psi(p) = \frac{1}{\sqrt{2L}} \cdot \frac{1}{\sqrt{2\pi\hbar}} \int_{-L}^{L} dx\, e^{-ipx/\hbar} = \frac{1}{2} \cdot \frac{1}{\sqrt{\pi L \hbar}} \cdot \left. \frac{e^{-ipx/\hbar}}{-ip/\hbar} \right|_{-L}^{L}$$

$$= -\sqrt{\frac{\hbar}{\pi L}} \cdot \frac{1}{p} \cdot \frac{1}{2i} \left(e^{-ipL/\hbar} - e^{ipL/\hbar} \right)$$

$$= \sqrt{\frac{L}{\pi\hbar}} \cdot \frac{1}{\frac{pL}{\hbar}} \cdot \sin\left(\frac{pL}{\hbar}\right)$$

Gustoća vjerojatnosti: $|\psi(p)|^2 = \rho(p)$

$$\rho(p) = \frac{L}{\pi\hbar} \cdot \frac{1}{\left(\frac{pL}{\hbar}\right)^2} \sin^2\left(\frac{pL}{\hbar}\right)$$

Da li je
$$\int_{-\infty}^{\infty} \rho(p)\, dp = 1 \ ?$$

$$\frac{pL}{\hbar} = \eta \ ; \quad dp = \frac{\hbar}{L} d\eta$$

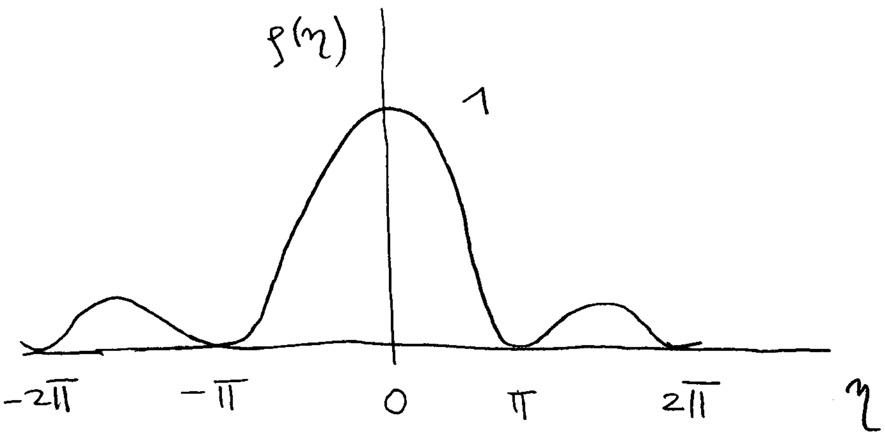
$$\int_{-\infty}^{\infty} \frac{L}{\pi\hbar} \cdot \frac{1}{\eta^2} \sin^2\eta \cdot \frac{\hbar}{L} d\eta = \frac{1}{\pi} \underbrace{\int_{-\infty}^{\infty} \frac{1}{\eta^2} \sin^2\eta \, d\eta}_{=\pi} = 1 \ \checkmark$$

(b) Gustoću $\rho(p)$ možemo nacrtati uvedemo li

$$\eta \equiv \frac{pL}{\hbar}$$

$$\rho(\eta) = \frac{\rho(p)}{\frac{L}{\pi\hbar}} \quad ; \quad \rho(\eta) = \frac{1}{\eta^2}\sin^2\eta$$

Drugim riječima, $\rho(p)$ čitamo u jedinicama $\frac{L}{\pi\hbar}$, a p čitamo u jedinicama $\frac{\hbar}{L}$



Neodređenost za x je

$$\Delta x \sim L$$

Neodređenost za p je

$$\Delta\eta \sim \pi \Rightarrow \Delta p \sim \pi \cdot \frac{\hbar}{L}$$

Imamo

$$\Delta x \cdot \Delta p \sim L \cdot \pi \frac{\hbar}{L} = \pi\hbar > \hbar$$

$$\Delta x \cdot \Delta p \gtrsim \hbar$$

Relacija neodređenosti za x i p je zadovoljena!

(c)
$$\rho_1 = \rho\left(\frac{h}{4L}\right) = \frac{L}{\pi\hbar} \cdot \frac{1}{\left(\frac{h}{4L}\cdot\frac{L}{\hbar}\right)^2} \sin^2\left(\frac{h}{4L}\cdot\frac{L}{\hbar}\right)$$

$$\rho_1 = \frac{L}{\pi\hbar} \cdot \frac{1}{\left(\frac{\pi}{2}\right)^2} \underbrace{\sin^2\left(\frac{\pi}{2}\right)}_{=1} = \frac{4L}{\pi^3\hbar}$$

$$\rho(0) = \lim_{p\to 0} \frac{L}{\pi\hbar} \cdot \frac{1}{\left(\frac{pL}{\hbar}\right)^2} \cdot \sin^2\left(\frac{pL}{\hbar}\right) = \frac{L}{\pi\hbar}$$

Imamo

$$\frac{\rho_1}{\rho(0)} = \frac{4}{\pi^2}$$

$\boxed{8.2}$

Valne funkcije za beskonačnu potencijalnu jamu širine L

$$\psi_n(x,t) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{n\pi}{L}x\right) e^{-iE_n t/\hbar}$$

Valne funkcije za beskonačnu potencijalnu jamu iz impulsnog prostora

$$\phi_n(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_0^L dx\, \psi_n(x,t)\, e^{-i\frac{p\cdot x}{\hbar}}$$

$$t=0;\quad \phi_n(p) = \frac{1}{\sqrt{2\pi\hbar}}\cdot\sqrt{\frac{2}{L}}\int_0^L dx\, \underbrace{\sin\left(\frac{n\pi}{L}x\right)}_{\frac{\left(e^{i\frac{n\pi}{L}x} - e^{-i\frac{n\pi}{L}x}\right)}{2i}} e^{-i\frac{p\cdot x}{\hbar}}$$

$$= \sqrt{\frac{1}{\pi\hbar L}}\cdot\frac{1}{2i}\int_0^L dx \left\{ e^{i\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)\cdot x} - e^{-i\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)x} \right\}$$

$$\int_0^L dx\, e^{i\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)x} = \frac{1}{i\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)}\, e^{i\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)x}\Big/_0^L$$

$$= \frac{1}{i\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)}\left\{ e^{i\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)L} - 1\right\}$$

$$\int_0^L dx\, e^{-i\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)x} = \frac{1}{-i\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)}\left\{ e^{-i\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)L} - 1\right\}$$

$$\phi_n(p) = \frac{1}{\sqrt{\pi\hbar L}}\cdot\frac{1}{2}\cdot\left\{ \frac{1}{\left(\frac{p}{\hbar}-\frac{n\pi}{L}\right)}\left[e^{i\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)L} - 1\right] - \frac{1}{\left(\frac{p}{\hbar}+\frac{n\pi}{L}\right)}\left[e^{-i\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)L} - 1\right]\right\}$$

$$\Phi_n(p) = \frac{1}{2}\cdot\frac{1}{\sqrt{\pi\hbar L}}\cdot\frac{1}{\left(\frac{p}{\hbar}\right)^2-\left(\frac{n\pi}{L}\right)^2}\cdot\left\{\left(\frac{p}{\hbar}+\frac{n\pi}{L}\right)\left(e^{i\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)L}-1\right)\right.$$

$$\left. -\left(\frac{p}{\hbar}-\frac{n\pi}{L}\right)\left(e^{-i\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)L}-1\right)\right\}$$

$$e^{i\frac{n\pi}{L}\cdot L} = e^{in\pi} = (-1)^n$$

$$\Phi_n(p) = \frac{1}{2}\cdot\frac{1}{\sqrt{\pi\hbar L}}\cdot\frac{1}{\left(\frac{p}{\hbar}\right)^2-\left(\frac{n\pi}{L}\right)^2}\cdot\left\{(-1)^n e^{-i\frac{pL}{\hbar}}\left(\frac{p}{\hbar}+\frac{n\pi}{L}\right)\right.$$

$$\left. -(-1)^n\left(\frac{p}{\hbar}-\frac{n\pi}{L}\right)e^{-i\frac{pL}{\hbar}} - \frac{2n\pi}{L}\right\}$$

$$= \frac{1}{2}\cdot\frac{1}{\sqrt{\pi\hbar L}}\cdot\frac{1}{\left(\frac{p}{\hbar}\right)^2-\left(\frac{n\pi}{L}\right)^2}\cdot\left\{(-1)^n e^{-i\frac{pL}{\hbar}}\cdot\frac{2n\pi}{L} - \frac{2n\pi}{L}\right\}$$

$$= \frac{n\pi}{L}\cdot\frac{1}{\sqrt{\pi\hbar L}}\cdot\frac{1}{\left(\frac{p}{\hbar}\right)^2-\left(\frac{n\pi}{L}\right)^2}\left\{(-1)^n e^{-i\frac{pL}{\hbar}}-1\right\}$$

$$\Phi_n(p,t) = \frac{n\pi}{L}\cdot\frac{1}{\sqrt{\pi\hbar L}}\cdot\frac{1}{\left(\frac{p}{\hbar}\right)^2-\left(\frac{n\pi}{L}\right)^2}\cdot\left\{(-1)^n e^{-i\frac{pL}{\hbar}}-1\right\}e^{-i\frac{E_n t}{\hbar}}$$

Ako je $p = \frac{n\pi}{L}\hbar$, tada

$$\Phi_n(p) = \frac{1}{\sqrt{\pi\hbar L}}\cdot\frac{1}{2i}\int_0^L dx\left\{1-e^{-i\frac{2n\pi}{L}x}\right\} =$$

$$= \frac{1}{\sqrt{\pi\hbar L}}\cdot\frac{1}{2i}\left\{L - \frac{e^{-i\frac{2n\pi}{L}x}}{\left(-\frac{2n\pi}{L}\right)}\Bigg/_0^L\right\}$$

$$= \frac{1}{\sqrt{\pi\hbar L}}\cdot\frac{1}{2i}\left\{L+\frac{L}{2n\pi}\cdot(1-1)\right\} = \frac{L}{2i}\cdot\frac{1}{\sqrt{\pi\hbar L}}$$

$$= \frac{1}{2\sqrt{\pi}\,i}\cdot\sqrt{\frac{L}{\hbar}}$$ → konačno pa je i $|\Phi_n(p)|^2$ konačno

$$\rho_n(p) = |\Phi_n|^2$$

$$= \frac{n^2\pi^2}{L^2} \cdot \frac{1}{\pi\hbar L} \cdot \frac{1}{\left[\left(\frac{p}{\hbar}\right)^2 - \left(\frac{n\pi}{L}\right)^2\right]^2} \cdot \left\{(-1)^n e^{-i\frac{pL}{\hbar}} - 1\right\}$$

$$\cdot \left\{(-1)^n e^{i\frac{pL}{\hbar}} - 1\right\}$$

$$= \frac{n^2\pi}{\hbar L^3} \cdot \frac{1}{\left[\left(\frac{p}{\hbar}\right)^2 - \left(\frac{n\pi}{L}\right)^2\right]^2} \cdot \left\{1 - (-1)^n \underbrace{\left(e^{-i\frac{pL}{\hbar}} + e^{i\frac{pL}{\hbar}}\right)}_{2\cos\left(\frac{pL}{\hbar}\right)} + 1\right\}$$

$$= \frac{2\pi n^2}{\hbar L^3} \cdot \frac{1}{\left[\left(\frac{p}{\hbar}\right)^2 - \left(\frac{n\pi}{L}\right)^2\right]^2} \cdot \left\{1 - (-1)^n \cdot \cos\left(\frac{pL}{\hbar}\right)\right\}$$

$\boxed{8.3}$

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

$$\langle x'|p|\alpha\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'|\alpha\rangle$$

$$\langle x'|H|\alpha\rangle = \frac{1}{2m}\langle x'|p^2|\alpha\rangle + \langle x'|V(x)|\alpha\rangle$$

Računamo matrični element $\langle x'|p^2|\alpha\rangle$

$$\langle x'|p^2|\alpha\rangle = \langle x'|p\, I\, p|\alpha\rangle = \left[I = \int dx\, |x\rangle\langle x| \right]$$

$$= \int dx\, \langle x'|p|x\rangle\langle x|p|\alpha\rangle$$

$$= \int dx\, \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'|x\rangle \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\alpha\rangle$$

$\langle x'|x\rangle = \delta(x-x')$ ortogonalnost vlastitih vektora

$\langle x|\alpha\rangle = \psi(x)$

$$= \int dx \left(\frac{\hbar}{i}\right)^2 \frac{\partial}{\partial x'}\delta(x-x')\,\frac{\partial\psi}{\partial x}$$

$$\frac{\partial}{\partial x'}\delta(x-x') = \delta'(x-x')\cdot(-1) = -\frac{\partial}{\partial x}\delta(x-x')$$

Svojstvo delta funkcije: $\int \frac{d}{dx}\delta(x-x')\, f(x)\, dx = -f'(x')$

$$= -\hbar^2 \frac{\partial^2\psi}{\partial x'^2}$$

Računamo matrični element $\langle x'|V(x)|\alpha\rangle$. Znamo da je

$$x|x'\rangle = x'|x\rangle$$

Ako je $V(x)$ analitička vrijedi

$$V(x)|x'\rangle = V(x')|x'\rangle$$

$$\langle x'|V(x)|\alpha\rangle = (\langle x'|V^+(x))\cdot|\alpha\rangle = V(x')\langle x'|\alpha\rangle$$

$$= V(x')\,\psi(x')$$

Dobijemo

$$\langle x'|H|\alpha\rangle = \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x')}{\partial x'^2} + V(x')\psi(x')$$

što smo, uobičajno u valnoj mehanici pisali kao

$$H\psi$$

Ako je $|\alpha\rangle$ svojstveni vektor od H

$$H|\alpha\rangle = \lambda|\alpha\rangle$$

S druge strane je

$$\begin{aligned}\langle x'|H|\alpha\rangle &= \langle x'|\cdot\left(H|\alpha\rangle\right) = \langle x'|\cdot\left(\lambda|\alpha\rangle\right)\\ &= \lambda\langle x'|\alpha\rangle\\ &= \lambda\psi(x')\end{aligned}$$

Sve skupa

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

što je jednadžba svojstvenih vrijednosti za H i $\psi(x')$ je svojstvena funkcija.

8.4

Označimo valnu funkciju iz impulsnog prostora s

$$\phi(p) = \langle p|\alpha\rangle$$

Ako je $|\alpha\rangle$ vlastiti vektor od H

$$H|\alpha\rangle = \lambda|\alpha\rangle$$

tada je $\phi(p)$ vlastita funkcija od H u p-reprezentaciji.

Računamo matrični element $\langle p'|H|\alpha\rangle$. Na jednoj strani

$$\langle p'|H|\alpha\rangle = \langle p'|\cdot\left(H|\alpha\rangle\right) = \lambda\langle p'|\alpha\rangle$$
$$= \lambda\,\phi(p')$$

Na drugoj strani

$$\langle p'|\left(\frac{p^2}{2m} + V(x)\right)|\alpha\rangle = \frac{1}{2m}\langle p'|p^2|\alpha\rangle + \langle p'|V(x)|\alpha\rangle$$

Računamo matrični element $\langle p'|p^2|\alpha\rangle$

$$\langle p'|p^2|\alpha\rangle = \left(\langle p'|(p^+)^2\right)\cdot|\alpha\rangle = p'^2\langle p'|\alpha\rangle$$

jer je

$$p|p'\rangle = p'|p'\rangle \quad i \quad \langle p'|p^+ = p'\langle p'|$$

$$\langle p'|V(x)|\alpha\rangle = \langle p'|I\cdot V(x)\cdot I|\alpha\rangle$$
$$= \int dx'\int dp'' \langle p'|x'\rangle\langle x'|V(x)|p''\rangle\langle p''|\alpha\rangle$$

$$\langle p'|x'\rangle = \left(\langle x'|p'\rangle\right)^* = \frac{1}{\sqrt{2\pi\hbar}}\, e^{-i\frac{p'x'}{\hbar}}$$

$$\langle x'|V(x)|p''\rangle = \left(\langle x'|V(x)\right)\cdot|p''\rangle = V(x')\langle x'|p''\rangle$$

$$\langle p'|V(x)|\alpha\rangle = \frac{1}{2\pi\hbar}\int dx'\int dp''\, e^{-i\frac{(p'-p'')\cdot x'}{\hbar}}\, V(x')\,\phi(p'')$$

Fourierov transformat od $V(x')$

$$V(p'-p'') = \frac{1}{\sqrt{2\pi\hbar}} \int dx' \, e^{-i\frac{(p'-p'')\cdot x'}{\hbar}} V(x')$$

Stoga je

$$\langle p'| V(x) |\alpha\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dp'' \, V(p'-p'') \, \phi(p'')$$

Dobijemo

$$\frac{p'^2}{2m} \phi(p') + \frac{1}{\sqrt{2\pi\hbar}} \int dp'' \, V(p'-p'') \, \phi(p'') = \mathcal{E} \phi(p')$$

što je traženi rezultat.

$\boxed{8.5}$

Operator položaja $\hat{x}$ djeluje na valnu funkciju tako da je pomnoži s x

$$\hat{x}\,\psi(x) = x\,\psi(x)$$

Ovo možemo zapisati pomoću ket-bra notacije ovako:

$$\langle x|\hat{x}|\alpha\rangle = (\langle x|\hat{x})\cdot|\alpha\rangle = (x\langle x|)\cdot|\alpha\rangle$$
$$= x\langle x|\alpha\rangle$$

gdje je $|x\rangle$ svojstveni vektor, a x svojstvena vrijednost za $\hat{x}$. Budući je $\psi(x) \equiv \langle x|\alpha\rangle$ vidimo da je

$$\hat{x}\,\psi(x) \leftrightarrow \langle x|\hat{x}|\alpha\rangle$$

Vektor $|\alpha\rangle$ je po volji odabran vektor stanja, pa odaberemo

$$|\alpha\rangle = |x'\rangle$$

Imamo

$$\langle x|\hat{x}|x'\rangle = \langle x|\cdot(\hat{x}|x'\rangle) = \langle x|\cdot(x'|x'\rangle)$$
$$= x'\langle x|x'\rangle = x'\,\delta(x-x')$$

Posljednja jednakost slijedi iz ortogonalnosti svojstvenih vektora $|x\rangle$ i $|x'\rangle$. Dobivamo:

$$\begin{array}{c} \langle x|\hat{x}|x'\rangle \leftrightarrow \hat{x}\,\delta(x-x') \\ \| \\ x'\,\delta(x-x') \end{array}$$

Sve skupa,

$$\hat{x}\,\delta(x-x') = x'\,\delta(x-x')$$

pa je $\delta(x-x')$ svojstvena funkcija za $\hat{x}$ sa svojstvenom vrijednošću x'.

$\boxed{8.6}$

Koristit ćemo relacije potpunosti

$$\int dp'' \, |p''\rangle\langle p''| = \mathbb{1}$$

$$\int dx' \, |x'\rangle\langle x'| = \mathbb{1}$$

$$\langle p'|x|\alpha\rangle = \int dp'' \langle p'|x|p''\rangle\langle p''|\alpha\rangle$$

$$= \int dp'' \int dx' \, \langle p'|x|x'\rangle\langle x'|p''\rangle\langle p''|\alpha\rangle$$

No, jednadžba svojstvenih vrijednosti za operator položaja x daje

$$x|x'\rangle = x'|x'\rangle$$

Također,

$$\langle x'|p''\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ix'p''/\hbar}$$

Imamo

$$\langle p'|x|\alpha\rangle = \int dx' \int dp'' \frac{x'}{2\pi\hbar} e^{-ix'p'/\hbar} \cdot e^{ix'p''/\hbar} \overbrace{\langle p''|\alpha\rangle}^{\Phi(p'')}$$

$$= \frac{1}{2\pi\hbar} \int dp'' \, \Phi(p'') \int dx' \frac{\partial}{\partial p''} \left[e^{ix'(p''-p')/\hbar} \cdot (-i)\hbar \right]$$

Diracova delta funkcija definirana je izrazom

$$\int_{-\infty}^{\infty} dx' \, e^{ix'(p''-p')/\hbar} = 2\pi\hbar \, \delta(p''-p')$$

Imamo

$$\langle p'|x|\alpha\rangle = \frac{\hbar}{i}\int dp''\, \Phi(p'')\, \frac{d}{dp''}\, \delta(p''-p')$$

Koristimo svojstvo Diracove delta-funkcije

$$\int f(x)\, \frac{d}{dx}\, \delta(x-x')\, dx = -\frac{d f(x')}{dx'}$$

Prema tome,

$$\langle p'|x|\alpha\rangle = -\frac{\hbar}{i}\frac{\partial}{\partial p'}\Phi(p')$$