Kanonické kvantování

$QM \Rightarrow CM \qquad \hbar \to 0$

$CM \Rightarrow QM$

Jak upravit existující klasickou teorii nějakého jevu, abych obdržel odpovídající kvantovou teorii?

$\Rightarrow$ Kanonické kvantování

veličiny $A, B \longrightarrow$ operátory $\hat{A}, \hat{B}$

klasické Poissonovy závorky $\{A, B\}$ — komutátory $[\hat{A}, \hat{B}]$

kanonicky sdružené veličiny, např. p a q — $\hat{p}, \hat{q}$

$$[\hat{q}, \hat{p}] \neq 0$$

$$\{A, B\} = C \quad \Rightarrow \quad [\hat{A}, \hat{B}] = i\hbar\hat{C}$$

Př:

$$\{p, q\} = \frac{\partial p}{\partial q}\frac{\partial q}{\partial p} - \frac{\partial p}{\partial p}\frac{\partial q}{\partial q} = -1 \Rightarrow [\hat{p}, \hat{q}] = -i\hbar$$

Ehrenfestův teorém

Pohybové rovnice pro střední hodnoty souřadnice a impulsu

$$\langle x(t)\rangle = \langle \psi(t)|\hat{x}|\psi(t)\rangle = \langle \psi(t_0)|\hat{U}^+(t,t_0)\,\hat{x}\,\hat{U}(t,t_0)|\psi(t_0)\rangle$$

$$\langle p(t)\rangle = \langle \psi(t)|\hat{p}|\psi(t)\rangle = \langle \psi(t_0)|\hat{U}^+(t,t_0)\,\hat{p}\,\hat{U}(t,t_0)|\psi(t_0)\rangle$$

$$\frac{d}{dt}\langle x(t)\rangle = \langle \psi(t_0)|\left(\frac{d}{dt}\hat{U}^+(t,t_0)\right)\hat{x}\,\hat{U}(t,t_0)|\psi(t_0)\rangle$$

$$+\langle \psi(t_0)|\hat{U}^+(t,t_0)\,\hat{x}\left(\frac{d}{dt}\hat{U}(t,t_0)\right)|\psi(t_0)\rangle$$

$$U(t,t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}$$

$$\frac{d}{dt}U(t,t_0) = -\frac{i}{\hbar}H\,U(t,t_0)$$

$$= \langle \psi(t_0)|\frac{i}{\hbar}\hat{H}\,\hat{U}^+(t,t_0)\,\hat{x}\,\hat{U}(t,t_0)|\psi(t_0)\rangle$$

$$-\frac{i}{\hbar}\langle \psi(t_0)|\hat{U}^+(t,t_0)\,\hat{x}\,\hat{H}\,\hat{U}(t,t_0)|\psi(t_0)\rangle$$

$$= \frac{i}{\hbar}\langle \psi(t)|\left(\hat{H}\hat{x}-\hat{x}\hat{H}\right)|\psi(t)\rangle$$

$$= \frac{i}{\hbar}\langle \psi(t)|\,[\hat{H},\hat{x}]\,|\psi(t)\rangle$$

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

$$[V(\hat{x}),\hat{x}] = 0$$

$$[\hat{x},\hat{p}] = i\hbar \rightarrow \hat{x}\hat{p} = \hat{p}\hat{x} + i\hbar$$

$$\left[\frac{\hat{p}^2}{2m},\hat{x}\right] = \frac{1}{2m}\left(\hat{p}^2\hat{x} - \hat{x}\hat{p}^2\right) =$$

$$= \frac{1}{2m}\left(\hat{p}\left(\cancel{\hat{x}\hat{p}}-i\hbar\right) - \left(\cancel{\hat{p}\hat{x}}+i\hbar\right)\hat{p}\right)$$

$$= -\frac{i\hbar}{m}\hat{p}$$

$$\boxed{\frac{d}{dt}\langle x(t)\rangle} = \frac{i}{\hbar}\left(-\frac{i\hbar}{m}\right)\langle\hat{p}\rangle = \boxed{\frac{\langle\hat{p}\rangle}{m}} \Rightarrow \dot{x} = \frac{p}{m}$$

Pohybová rovnice pro $\langle p(t) \rangle$

$$\boxed{\frac{d}{dt}\langle p(t)\rangle} = \ \dots \ = \frac{i}{\hbar}\langle \psi(t)|[\hat{H},\hat{p}]|\psi(t)\rangle$$

$$= \frac{i}{\hbar}\langle \psi(t)|[\hat{V}(\hat{q}),\hat{p}]|\psi(t)\rangle$$

$$= \frac{i}{\hbar}\langle \psi(t)|\, i\hbar \frac{d\hat{V}(\hat{q})}{d\hat{q}}\, |\psi(t)\rangle = \boxed{-\left\langle \frac{d\hat{V}(q)}{dq}\right\rangle}$$

opět jako v klasické mechanice

$$\hat{V}(\hat{q}) = V_0 + V_1\hat{q} + V_2\hat{q}^2 + \dots$$

$$[V_0,\hat{p}] = 0$$

$$V_1[\hat{q},\hat{p}] = i\hbar V_1 \quad \dots$$

z komutační relace $[\hat{p},\hat{q}]$