QMI-7 Časový vývoj v QM

Minule: $|\psi(t)\rangle = \hat{U}(t)|\psi_0\rangle$ $\qquad i\hbar\,\partial_t|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$

- $i\hbar\,\partial_t \hat{U}(t) = \hat{H}(t)\hat{U}(t)$ differential Schrödinger equation
- $\hat{U}(t) = \hat{I} + \frac{1}{i\hbar}\int_0^t \hat{H}(\tau)\hat{U}(\tau)\,d\tau$ integral (1) Dyson equation

iterace: $\hat{U}(t) = \sum_n \left(\frac{1}{i\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n\, \hat{H}(t_1)\hat{H}(t_2)\dots\hat{H}(t_n)$

Operátor časového uspořádání:

$$T\,\hat{H}(t_1)\hat{H}(t_2)\dots\hat{H}(t_n) = T\,\hat{H}(t_n)\dots\hat{H}(t_1) = \hat{H}(t_{i_1})\dots\hat{H}(t_{i_n})$$

$$t_{i_1} \le t_{i_2} \le \dots \le t_{i_n}$$

$$\rightarrow \hat{U}(t) = T\sum_n \frac{1}{n!}\left[\frac{1}{i\hbar}\int_0^t \hat{H}(\tau)\,d\tau\right]^n \equiv T\exp\left\{-\frac{i}{\hbar}\int_0^t \hat{H}(\tau)\,d\tau\right\}$$

- spec. případ $[\hat{H}(t_1),\hat{H}(t_2)]=0$ vypustím $\qquad H=\text{konst} \dots \hat{H}t$

Časový vývoj pro bodovou částic

- ... $\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{x})$ ... (SR) => $\qquad \partial_t\rho + \operatorname{div}\vec{j} = 0$ (2)

kde $\rho(x) = \psi^*(x)\psi(x)$ $\qquad \dots\ \vec{j} = -\frac{i\hbar}{2m}[\psi^*\nabla\psi - \psi\nabla\psi^*] = \frac{\hbar}{m}\operatorname{Im}\psi^*\nabla\psi$

hustota toku pravděpodobnosti

(3) Greenův operátor Schrödingerovy rovnice:

Retardovaný $\qquad \hat{G}^{(+)}(t_2,t_1) = \theta(t_2-t_1)\,\hat{U}(t_2,t_1)$

Advancovaný $\qquad \hat{G}^{(-)}(t_2,t_1) = -\theta(t_1-t_2)\,\hat{U}(t_2,t_1)$

$$\rightarrow \left[i\hbar\,\partial_{t_2} - \hat{H}\right]\hat{G}(t_2,t_1) = i\hbar\,\delta(t_1-t_2)$$

$$\hat{U} = e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}(t_2-t_1)}$$

Propagátor (volné částice):

$$\hat{G}_0^{(+)}(\vec{x}_2,t_2,\vec{x}_1,t_1) = \langle\vec{x}_2|\hat{G}_0^{(+)}(t_2,t_1)|\vec{x}_1\rangle$$

$$G_{3D} = G_x\cdot G_y\cdot G_z$$

$$= \theta(t_2-t_1)\left[\frac{m}{2\pi\hbar i(t_2-t_1)}\right]^{3/2}\exp\left\{\frac{im}{2\hbar}\frac{(\vec{x}_2-\vec{x}_1)^2}{t_2-t_1}\right\},$$

4) Pohyb vlnového balíku (klubka) .. bodová částice

$x \in (-\infty, \infty)$

pozn: minimalizující vlnový balík .. $\boxed{\Delta x \cdot \Delta p \geq \frac{\hbar}{2}}$

$$\psi(x) = \frac{1}{\sqrt{\Delta\sqrt{2\pi}}} e^{-\left(\frac{x}{2\Delta}\right)^2}$$

$$\|\psi\|^2 = \int_{-\infty}^{\infty} e^{-\frac{1}{2}\left(\frac{x}{\Delta}\right)^2} dx = \sqrt{2\pi} \cdot \Delta$$

$$I(a) = \int e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \quad -\frac{1}{2}\sqrt{\frac{\pi}{a}}\frac{1}{a}$$

$$I' = -\int x^2 e^{-ax^2}$$

$\langle x \rangle = 0 \qquad \langle p \rangle = 0$

$$\Delta x^2 = \int_{-\infty}^{\infty} \frac{x^2}{\Delta^2} e^{-\frac{1}{2}\left(\frac{x}{\Delta}\right)^2} \frac{dx}{\Delta} \frac{\Delta^3}{\Delta\sqrt{2\pi}} = \frac{\Delta^2}{\sqrt{2\pi}} \cdot \frac{1}{2}\sqrt{2\pi} \cdot 2$$

$$\int y^2 e^{-ay^2} dy$$

$\boxed{\Delta_x = \Delta}$

$$\frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px}$$

$$\psi(p) = \int \langle p|x\rangle \psi(x) dx$$

$$= \frac{1}{\sqrt{\Delta_x\sqrt{2\pi}}} \int \frac{dx}{\sqrt{2\pi\hbar}} e^{-\left(\frac{x}{2\Delta_x}\right)^2 - \frac{i}{\hbar}p\Delta_x 2 \frac{x}{2\Delta_x} - \left(\frac{i}{\hbar}p\Delta_x\right)^2}$$

$$(A+B)^2 = A^2 + 2AB$$

$$e^{-\left(\frac{p\Delta x}{\hbar}\right)^2} \quad \left(\frac{p}{2\Delta_p}\right)^2$$

$$\boxed{\Delta_p = \frac{\hbar}{2\Delta_x}}$$

$$\frac{1}{\sqrt{\Delta_x\sqrt{2\pi}}} \frac{1}{(2\pi\hbar)} e^{-\left(\frac{p}{2\Delta_p}\right)^2} \underbrace{\int e^{-\frac{1}{4\Delta_x^2}(x + \text{něco})^2} dx}_{\sqrt{\pi} \cdot 2\Delta x} = \frac{1}{\sqrt{\Delta p\sqrt{2\pi}}} e^{-\left(\frac{p}{2\Delta_p}\right)^2}$$

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přehled Gauss-minimální balíky

x-reprezentace

$$\psi(x) = \frac{1}{\sqrt{\Delta_x\sqrt{2\pi}}} e^{-\left(\frac{x-x_0}{2\Delta_x}\right)^2} e^{\frac{i}{\hbar}p_0 x}$$

$\langle \hat{x} \rangle = x_0 \qquad \Delta_x^2 = \langle x^2 \rangle - \langle x \rangle^2$

$\ldots \psi(\vec{x}) = \psi_x \cdot \psi_y \cdot \psi_z \quad \ldots \Delta_x, \Delta_y, \Delta_z$

p-reprezentace

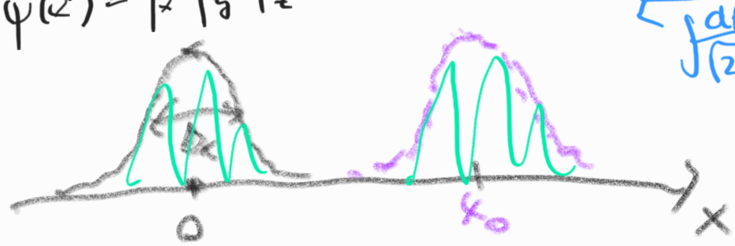
$\boxed{\Delta_x \Delta_p = \hbar/2}$

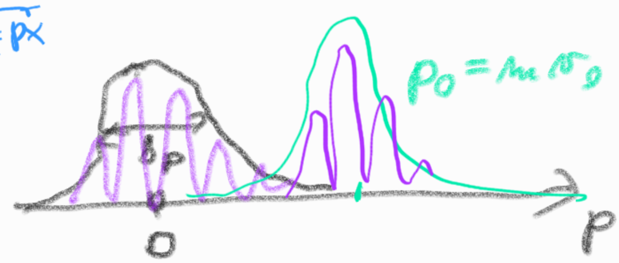
$$\psi(p) = \frac{1}{\sqrt{\Delta_p\sqrt{2\pi}}} e^{-\left(\frac{p-p_0}{2\Delta_p}\right)^2} e^{-\frac{i}{\hbar}px_0}$$

$\langle \hat{p} \rangle = p_0 \qquad \Delta_p^2 = \langle p^2 \rangle - \langle p \rangle^2$

$$\int \frac{dx}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px}$$

$$\int \frac{dp}{\sqrt{2\pi\hbar}} e^{+\frac{i}{\hbar}px}$$





časový vývoj: (i) $G_0^{(+)}$: $\psi(x_2, t_2) = \int d^3x_1 \, G_0^{(+)}(x_2 t_2, x_1 t_1) \psi(x_1, t_1)$

(ii) $|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht} \psi_0 \underset{p\text{-repr.}}{=} e^{-\frac{i}{\hbar}\frac{p^2}{2m}t} \psi_0(p)$ $\quad p^2$

$$H = \frac{p^2}{2m}$$

$$\psi(x, t) = \int dp \, \langle x|p\rangle \psi(p)$$

xp

výsledek: $\forall t$ ~~$t>0$~~

$$\boxed{\psi(x,t) = \frac{1}{\sqrt{\Delta_x\sqrt{2\pi}}}\frac{1}{\sqrt{1+i\alpha}}\exp\left\{-\frac{(x-\mu_0\alpha)^2}{1+\alpha^2}\right\}\exp\left\{i\,\frac{\alpha(x^2-\mu_0^2)+2x\mu_0}{1+\alpha^2}\right\}}$$

$$x = \frac{x}{2\Delta_x}\qquad \mu = \frac{p}{2\Delta_p}\qquad \frac{\Delta_p}{m\Delta_x}\,t \equiv \alpha(t)$$

- $x_0 = 0$
- $p_0 \neq 0$ $\mu_0 = \frac{p_0}{2\Delta_p}$

$$\psi(x,t) = \int\frac{dp}{\sqrt{2\pi\hbar}}\,e^{-\frac{i}{\hbar}px}\,\frac{1}{\sqrt{\Delta_p\sqrt{2\pi}}}\,e^{-\left(\frac{p-p_0}{2\Delta_p}\right)^2}\cdot e^{-\frac{i}{\hbar}\frac{p^2}{2m}t}$$

srovn. $|\psi|^2$ G-balík

$$\frac{1}{\Delta_x\sqrt{2\pi}}\exp\left(-\frac{1}{2}\left(\frac{x-x_0}{\Delta_x}\right)^2\right)$$

interpretace:

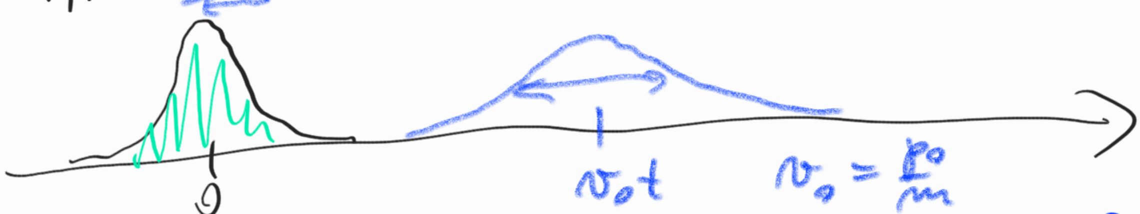
$$\rho(x,t) = \frac{1}{\sqrt{2\pi}}\,\frac{1}{\Delta_x\sqrt{1+\alpha^2}}\exp\left\{-2\,\frac{(x-\mu_0\alpha)^2}{(1+\alpha^2)}\right\}$$

$$-2\,\frac{\left(\frac{x}{2\Delta_x}-\frac{p_0}{2\Delta_p}\cdot\frac{\Delta_p}{m\Delta_x}t\right)^2}{1+\alpha^2} = -\frac{1}{2}\,\frac{\left(x-\frac{p_0}{m}t\right)^2}{\Delta_x^2(1+\alpha^2)}$$

$$\boxed{\Delta_x(t) = \Delta_x\sqrt{1+\alpha^2}}$$

- $\langle x(t)\rangle = \frac{p_0}{m}t = v_0 t$ $\quad t>0$ $\quad x_0 = 0$

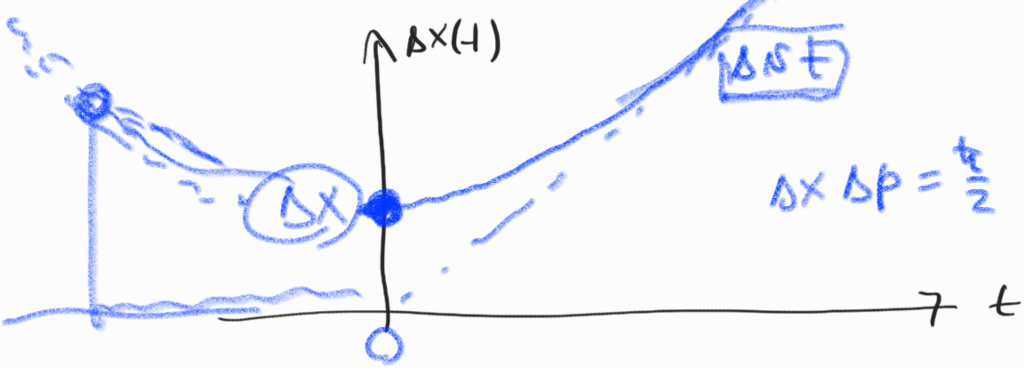
Fz7 $|\psi|^2$



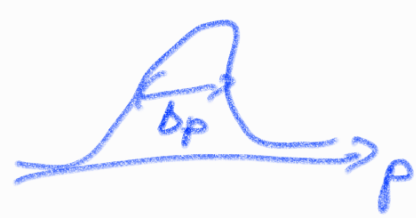
$$\Delta x(t)^2 = \Delta x^2(1+\alpha^2) = \Delta x^2\left(1+\left(\frac{\Delta p}{m\Delta x}\right)^2 t^2\right) = \Delta x^2 + \left(\frac{\Delta p}{m}t\right)^2$$

$(\Delta v t)^2$

$\Delta v \equiv \frac{\Delta p}{m}$



$\Delta x\,\Delta p = \frac{\hbar}{2}$



5) Časový vývoj v Haisenbergově obraze

(Haisenberg picture representation)

~~Až~~ sem ... Schrödingerův obraz $\quad|\psi(t)\rangle$ .. $\hat{A}$ (nezáv. na čase)

$|\psi_S(t)\rangle = U(t)\,|\psi_S(0)\rangle$ ... předp. H čas. nezáv. $\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}$

$$\langle A\rangle_t = \langle\psi_S(t)|\hat{A}_S|\psi_S(t)\rangle = \langle\psi_S(0)|\underbrace{\hat{U}^+(t)\,\hat{A}_S\,\hat{U}(t)}_{\hat{A}_H(t)}|\psi_S(0)\rangle$$

... $\partial_t A_S = 0$

$$\underline{p_a(t)} = \langle \psi_S(t) | \hat{P}_a | \psi_S(t) \rangle = \langle \psi_S(0) | P_a^{(H)}(t) | \psi_S(0) \rangle$$

$$P_a^{(S)} = \sum_\alpha |a\alpha\rangle\langle a\alpha| \qquad \hat{U}^+(t)\hat{P}_a^{(S)}\hat{U}(t) = \hat{P}_a^{(H)}$$

<u>Heisenbergův obraz:</u> $|\psi_H\rangle$ stavy nezávisí na čase

$$|\psi_S(t_0)\rangle \equiv |\psi_H(t_0)\rangle \qquad \text{BÚNO } t_0 = 0$$

měřitelné veličiny ... $A_H(t) = U^+(t) A_S U(t)$

Heisenbergova pohyb. rce: $\boxed{\frac{dA_H}{dt} = \frac{1}{i\hbar}[A_H(t), H]} \boxed{+\frac{\partial}{\partial t} A_H}$

$$\boxed{U^+ \frac{\partial}{\partial t} A_S U}$$

$$\frac{d}{dt} A_H = \frac{d}{dt} U^+ A_S U = \frac{1}{i\hbar}\left[U^+ A_S H U - U^+ H A_S U\right] \qquad (UU^+ = I) \quad (UU^+ = I)$$

$$\frac{d}{dt} U = \frac{1}{i\hbar} H U \qquad = \frac{1}{i\hbar}\left[A_H H - H A_H\right] = \frac{1}{i\hbar}[A_H, H]$$

$$\frac{d}{dt} U^+ = -\frac{1}{i\hbar} U^+ H$$

Hamilt. je stejný

$$H_H = U^+ H U = U^+ U H = H \quad \dots \quad H_S = H_H = H$$

$$[H, U] = [H, U^+] = 0$$

<u>pozn.</u> spektr. rozkl.: $A_S = \sum_a a P_a$

$$\underline{A_H = \sum_a a\, U^+ P_a U = \sum_a a\, P_a^{(H)}}$$

<u>pozn.</u> $\underline{(AB)_H} = U^+ A B U = U^+ A U \cdot U^+ B U = A_H B_H$

$$UU^+ = I \qquad U^+ I U = I$$

$$f(\hat{A})_H = f(\hat{A}_H) \qquad (A^n)_H = A_H^n$$

$$\underline{[x_H, p_H] = i\hbar I}$$

<u>PŘ.</u> částice $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(x)$

$$\rightarrow \dot{x}_H = \frac{1}{i\hbar}[\hat{x}_H, \hat{H}] = \frac{1}{i\hbar}\left[\hat{x}_H, \frac{p_H^2}{2m} + \cancel{V(x_H)}\right] = \frac{1}{i\hbar 2m}[x_H, p_H^2] = \frac{\hat{p}_H}{m} = \hat{v}_H$$

$$p[x,p] + [x,p]p \quad (i\hbar,\ i\hbar)$$

$$\dot{p}_H = \frac{1}{i\hbar}[p_H, \hat{H}] = \frac{1}{i\hbar}\left[p_H, \frac{p_H^2}{2m} + V(x_H)\right] = \frac{1}{i\hbar}[p_H, V(x_H)]$$

$$\frac{d}{dt}\hat{p}_H = -V'(\hat{x}_H) \qquad \dot{\hat{x}}_H = \frac{\hat{p}_H}{m} \qquad \dot{\hat{p}}_H = -V'(\hat{x}_H) \qquad \langle\psi_H| \quad |\psi_H\rangle$$

$V' \quad m\omega^2\hat{x}$

$V(\hat{x}) = \frac{1}{2}m\omega^2\hat{x}^2$

$\Rightarrow$ Ehrenfestův teorém

$$\langle\psi|\frac{dx}{dt}|\psi\rangle = \boxed{\frac{d}{dt}\langle x\rangle = \frac{\langle p\rangle}{m}}$$

$$\langle\psi|\frac{dp}{dt}|\psi\rangle \quad \boxed{\frac{d}{dt}\langle p\rangle = -\langle V'(x)\rangle} \overset{?}{\simeq} -V'(\langle x\rangle_H)$$

$$\langle V'(x)\rangle \neq V(\langle x\rangle)$$

PŘ: Volná částice tj $V=0$

Gauss balík:

$$\dot{x}_H = \frac{1}{i\hbar}[x_H, H] = \frac{p(t)}{m} = \text{konst} \longrightarrow \boxed{\hat{x}(t) = \hat{x}_S + \frac{\hat{p}_S}{m}t}$$

$$\dot{p}_H = -V'(x_H) = 0 \Longrightarrow p_H(t) = \hat{p}_S$$

$$\langle x(t)\rangle = \langle x(0)\rangle + \frac{\langle p_0\rangle}{m}t \quad \text{--- stejné co výše}$$

$$\Delta x(t)^2 = \langle x_H^2\rangle_t - \langle x_H\rangle_t^2$$

$$\langle(x_0 + \frac{p_0}{m}t)^2\rangle = \langle x_0^2\rangle + \frac{t}{m}\langle\hat{x}_0\hat{p}_0 + \hat{p}_0\hat{x}_0\rangle + \frac{t^2}{m^2}\langle p_0^2\rangle$$

$$\Delta x_t^2 = \Delta x_0^2 + \frac{\Delta p_0^2}{m^2}t^2 + \boxed{\frac{1}{m}\left(\langle xp+px\rangle_0 - 2\langle x\rangle_0\langle p\rangle_0\right)t}$$

dá se dk $=0$ pro minim. Gauss balík

$\boxed{x_0 = 0}$ jednoduše

PŘ: Lineární harm. oscilátor: $H = \frac{p^2}{2m} + \underbrace{\frac{1}{2}m\omega^2x^2}_{m\omega^2 x}$

Heisenberg pohyb: $\dot{x}_H = \frac{1}{i\hbar}[X_H, H] = \frac{p_H}{m}$

$\dot{p}_H = \frac{1}{i\hbar}[p_H, H] = -V'(x_H) = -m\omega^2 \hat{x}_H = -k\hat{x}_H$

$\omega = \sqrt{\frac{k}{m}}$

~ totožné klas Hamilt. rovnicím

Ehrenfest: $\frac{d}{dt}\langle x\rangle = \langle p\rangle / m = \langle v\rangle$, $\frac{d}{dt}\langle p\rangle = -k\langle x\rangle$ — stř. hodnoty splňují klas. pohyb. rovnice