QMI-4 | Bodová částice 1D

$\mathcal{H} = L^2(\mathbb{R})$

• x-reprezentace: $|\psi\rangle \longleftrightarrow \psi(x)$ $\qquad |x\rangle$

↳ ÚSKO .. $\hat{x}$ ... $\hat{x}\psi(x) = x\,\psi(x)$

další pozorovatelné $\qquad \hat{p}\psi(x) = -i\hbar \frac{d}{dx}\psi(x)$ $\qquad$ hybnost

$\rightarrow \phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}\hat{p}x}$

• p-reprezentace:

ÚSKO .. $\hat{p}$ $\qquad |\psi\rangle \longleftrightarrow \psi(p)$

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

$\hat{x}\psi(p) = i\hbar \frac{d}{dp}\psi(p)$

poloha

• ÚSKO .. $\hat{H}_0, \hat{P}$ $\qquad$ v x-repr.. $\qquad \hat{H}_0 = \frac{\hat{p}^2}{2m}$ -- kinet. energ.

$[H_0, P] = 0$ $\qquad$ Hamilt. volné částice

prostorová inverze (parita) $\qquad \hat{P}\psi(x) = \psi(-x)$

$\sigma_{H_0} = (0,\infty)$ .. vl. č. E $\rightarrow$ vl. v. $e^{\pm\frac{i}{\hbar}p_E x}$ $\qquad p_E = \sqrt{2mE}$

$\sigma_P = \{1,-1\}$ -- sudé/liché fce

SPOLEČNÉ vl. v. $|E,\lambda\rangle <$

$|E+\rangle \sim \cos\frac{p_E x}{\hbar} \sim \frac{n}{\sqrt{2}}(|p_E\rangle + |p_{-E}\rangle)$

$|E-\rangle \sim \sin\frac{p_E x}{\hbar} \sim \frac{n}{\sqrt{2}}(|p_E\rangle - |p_{-E}\rangle)$

normovací konstanta?

$$|E\lambda\rangle = \frac{n}{\sqrt{2}}(|p_E\rangle + \lambda|p_{-E}\rangle)$$

$\langle E\lambda|E'\lambda'\rangle = \delta_{\lambda\lambda'}\delta(E-E')$ $\qquad \langle p|p'\rangle = \delta(p-p')$

$\frac{|n|^2}{2}\left((\langle p_E| + \lambda\langle p_{-E}|)(|p_{E'}\rangle + \lambda'|p_{-E'}\rangle)\right)$ $\qquad \delta(p_E - p_{E'})$

$p_{E'} - p_E$

$= \frac{|n|^2}{2}\left\{\delta(p_E - p_{E'})\underbrace{[1+\lambda\lambda']}_{2\delta_{\lambda\lambda'}} + \underbrace{\delta(p_E + p_{E'})}_{0}[\lambda + \lambda']\right\}$

$p_E > 0$

$= |h^2|\,\delta_{\lambda\lambda'}\,\delta(p_E - p_E')$ $\quad p' = p_{E'}$ $\quad \delta(f(x)) = \sum_{x_0} \frac{\delta(x_0)}{|f'(x_0)|}$

$$\delta(E - E') = \delta\left(\frac{p^2}{2m} - \frac{p'^2}{2m}\right) = \frac{m}{p}\,\delta(p - p')$$

$E = \frac{p_E^2}{2m}$

ZÁVĚR:

$$\boxed{|E+\rangle = \sqrt{\frac{m}{\pi\hbar p}}\cos\frac{p_E x}{\hbar} \qquad |E-\rangle = \sqrt{\frac{m}{\pi\hbar p}}\sin\frac{p_E x}{\hbar}}$$

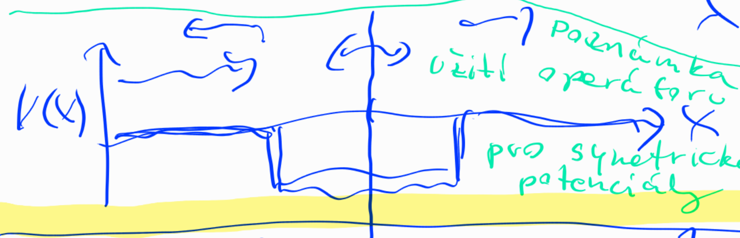
$p_E = \sqrt{2mE}$

společná ON báze operátorů $\hat H_0$ a $\hat P$

Příklad užití:

$$\hat U(t) = e^{-\frac{i}{\hbar}\hat H_0 t} = \sum_\lambda \int_0^\infty dE\, |E\lambda\rangle\langle E\lambda|\, e^{-\frac{i}{\hbar}Et}$$

výpočet evolučního operátoru



Poznámka užití operátoru $\hat P$ pro symetrické potenciály

$\psi_+(E), \psi_-(E)$ ...

struktura $|\psi\rangle$ v repr. $\{\hat H_0, \hat P\}$ $\quad \begin{pmatrix}\psi_+ \\ \psi_-\end{pmatrix}$

ČÁSTICE v pot.

$$\hat H = \hat H_0 + V(\hat x) = \frac{\hat p^2}{2m} + V(\hat x)$$

tvar $V(x)$:

1) konst. $V = V_0$ ... $\quad \hat H = \hat H_0 + V_0 \hat I \longrightarrow H_0$ $\quad E,\ V_0$ $\quad E' = E - V_0$

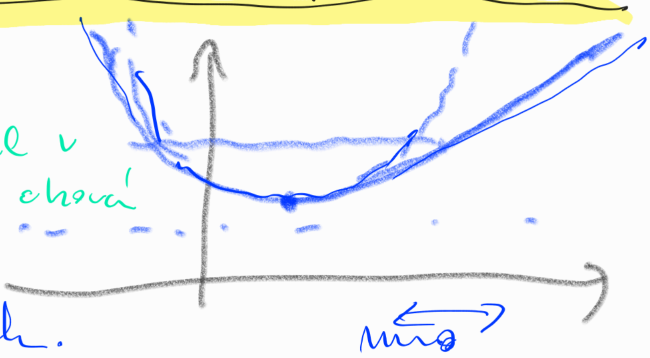
polynom 1. ř. $V = -Fx$

3) polynom 2. ř. v okolí minima: **Lineární harmonický oscilátor (LHO)**

univerzální model kmitů při nízké E

motivace

libovolný potenciál v okolí minima se chová jako LHO

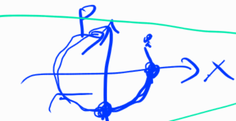


klasická mech.

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 \qquad \omega = \sqrt{\frac{k}{m}} \qquad T = \frac{2\pi}{\omega}$$

klasický pohyb: ve fázovém prostoru (kruh)

$$\left.\begin{aligned} \dot p &= -\frac{\partial H}{\partial x} = -kx \\ \dot x &= \frac{\partial H}{\partial p} = \frac{p}{m} \end{aligned}\right\} \xrightarrow{\text{řešení}} \begin{aligned} x &= x(0)\cos[\omega(t-\tau)] \\ p &= -m\omega x(0)\sin(\omega(t-\tau)) \end{aligned}$$

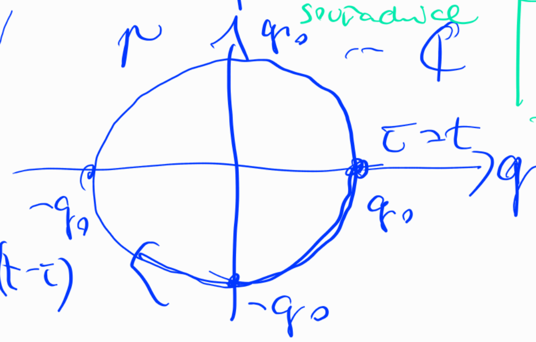


bezrozm veličiny: x -- $[\hbar] = \{x\,p\}$

$$\boxed{x_0 = \sqrt{\frac{\hbar}{m\omega}} \qquad p_0 = \frac{\hbar}{x_0}}$$

... bezrozm. souřadnice ... q

$$\boxed{q = \frac{x}{x_0}} \qquad \boxed{p = \frac{p}{p_0}}$$



- $q(t) = q_0 \cos\omega(t-\tau)$
- $p(t) = -q_0 \sin\omega(t-\tau)$

komplexní formalismus:

$$a(t) = \frac{1}{\sqrt{2}}(q + ip) = q_0 e^{-i\omega(t-\tau)}$$

$$\boxed{\hat{p} = p_0\hat{p} \\ \hat{x} = x_0\hat{q}}$$

- Kvantová mechanika

$$\boxed{\text{ÚSKO} \;..\; \hat{H}} \;..\; v\; L^2(\mathbb{R})$$

kde $\boxed{\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2}$ ← rozměrné

$H|\psi\rangle = E|\psi\rangle \quad E \in \sigma_H$

bezrozměrné

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{p}^2 + \hat{q}^2)$$

x-repres.	**p-repr.**
$\hat{q}$ ... q	... $\hat{p}$ ... p
$\hat{p}$ ... $-i\frac{\partial}{\partial q}$	... $\hat{q}$ ... $+i\frac{\partial}{\partial p}$
$= \frac{1}{2}\hbar\omega\left(-\frac{d^2}{dq^2} + q^2\right)$	$\frac{1}{2}\hbar\omega\left(p^2 - \frac{d^2}{dp^2}\right)$

stejný tvar

H

$$\boxed{\frac{1}{2}\hbar\omega\left(-\frac{d^2}{dq^2} + q^2\right)\psi(x) = E\,\psi(x)}$$

$$\hat{q} = \frac{\hat{x}}{x_0} \qquad \hat{p} = \frac{\hat{p}}{p_0} = \frac{x_0}{\hbar}(-i\hbar)\frac{d}{dx} = \frac{x_0}{\hbar}(-i\hbar)\frac{d}{x_0\,dq} = -i\frac{d}{dq}$$

Hledání σ_H -- vl. fce vl. č. $\hat{H}|\psi\rangle = E|\psi\rangle$

ALGEBRAICKÉ ŘEŠENÍ:

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{p}) \quad \text{anihilační operátor}$$

$$[\hat{x}, \hat{p}] = i\hbar\hat{I} \implies [\hat{q}, \hat{p}] = i\hat{I}$$

ladder operators

$$\hat{a}^+ = \frac{1}{\sqrt{2}}(\hat{q} - i\hat{p}) \quad \text{kreační operátor}$$

$$[\hat{a}, \hat{a}^+] = \frac{1}{2}[\hat{q} + i\hat{p}, \hat{q} - i\hat{p}]$$

$$\boxed{[\hat{a}, \hat{a}^+] = 1}$$

--- $\hat{N} = \hat{a}^+\hat{a}$ ... $\hat{N}^+ = \hat{N}$

$$\boxed{\hat H = \hbar\omega\left(\hat N + \tfrac{1}{2}\right)}$$

$$\hat N = \frac{1}{2}(\hat q - i\hat p)(\hat q + i\hat p) = \frac{1}{2}\Big[\hat q^2 + \hat p^2 + i\underbrace{(\hat q\hat p - \hat p\hat q)}_{i}\Big]$$

$$\hat N = \frac{\hat H}{\hbar\omega} - \frac{1}{2}$$

$$\boxed{\begin{aligned}[\hat N, \hat a] &= -\hat a\\ [\hat N, \hat a^+] &= a^+\end{aligned}}$$

$$\hat N|n\rangle = n|n\rangle$$

$$\hat N\hat a^+|n\rangle = \Big(\hat a^+\hat N + \underbrace{[\hat N, \hat a^+]}_{a^+}\Big)|n\rangle = \hat a^+|n\rangle\cdot n + \hat a^+|n\rangle = (n+1)\,\hat a^+|n\rangle$$

$$\to \underbrace{\hat a^+|n\rangle}_{|\psi\rangle} = C\,|n+1\rangle \qquad \big(N|\psi\rangle = (n+1)|\psi\rangle\big)$$

$$\hat N a|n\rangle = (\;\_\;\_\;\_\;)\,|n\rangle = (n-1)\,a|n\rangle$$

$$\hat a|n\rangle = C\,|n-1\rangle$$

normování $\langle\psi|\psi\rangle = \langle n|\underbrace{\hat a\hat a^+}|n\rangle = \langle n|(N+1)|n\rangle = n+1$ $\qquad (n+1)\langle n|n\rangle$

$|C|^2 \qquad \underbrace{a^+a}_{N} + \underbrace{[a, a^+]}_{I}$

$$\|\psi\|^2 = n+1$$

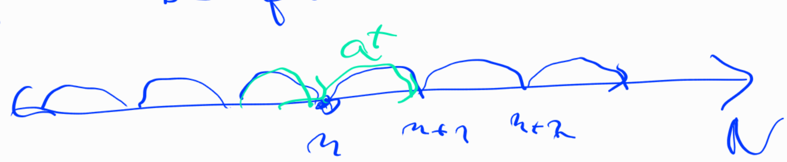
$$(*)\quad \boxed{\begin{aligned}\hat a^+|n\rangle &= \sqrt{n+1}\,|n+1\rangle\\ \hat a|n\rangle &= \sqrt{n}\,|n-1\rangle\end{aligned}} \quad \leftarrow \text{fáz konvence}$$

požadujeme aby (*) platily bez fáze

0

ladder property

$\mathbb{N}$ $\qquad n \in \sigma_N$



pozit. definitní $\quad \langle\psi|N|\psi\rangle = \langle\psi|a^+\underbrace{a|\psi\rangle}_{|\phi\rangle} = \|\phi\|^2 \geq 0$

$\Rightarrow$ n jsou celá nezáporná čísla

$\hat{a}\,|0\rangle = 0$ (SPECTRUM) -- $\sigma(\hat{n}) = \{0, 1, 2, 3, \dots\}$

$H = \hbar\omega(N + \frac{1}{2})$ -- $\sigma(\hat{H}) = \{E_n = \hbar\omega(n+\frac{1}{2})\}_{n=0}^{\infty}$

$|0\rangle$ -- $\langle q|\phi_0\rangle = \boxed{\phi_0(q)}$? najít

$|n\rangle = \frac{a^+}{\sqrt{n}} \dots \frac{a^+}{\sqrt{2}} \frac{a^+|0\rangle}{\sqrt{1}} = \frac{1}{\sqrt{n!}}(\hat{a}^+)^n|0\rangle$

$\boxed{\text{ÚSKO } \hat{H}_0}$

(Energet. repr. LHO)

$0 = \hat{a}\,|\phi\rangle = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{p})\phi_0(q) = \frac{1}{\sqrt{2}}\left(q + \frac{d}{dq}\right)\phi$, $\hat{p} = -i\frac{\partial}{\partial q}$

$q\,\phi(q) + \phi'(q) = 0$ $\quad \frac{\phi'}{\phi} = -q$ $\quad \ln\phi = -\frac{1}{2}q^2 + C$

$L^2 = \ell^2 \longrightarrow \boxed{\phi_0(q) = \frac{1}{\sqrt[4]{\pi}} e^{-\frac{1}{2}q^2}}$ $\quad \int_{-\infty}^{\infty}\phi^2 = \dots \sqrt{\pi}$

$x \quad p$ $\quad \begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ \vdots\end{pmatrix}$

$\Rightarrow$ ON báze v $\mathcal{H}$ -- $\{|n\rangle\}_{n=0}^{\infty}$

- reprezentace stavů -- $|\psi\rangle = \sum_{n=0}^{\infty} |n\rangle \underbrace{\langle n|\psi\rangle}_{\psi_n} = \sum_n \psi_n |n\rangle$
- měřitelné veličiny

$\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} + i\frac{\hat{p}}{p_0}\right)$ $\quad \hat{x} = \frac{x_0}{\sqrt{2}}(\hat{a} + \hat{a}^+)$ $\quad \hat{p} = \frac{p_0}{\sqrt{2}i}(\hat{a} - \hat{a}^+)$

$a^+ \quad -$

$\langle n'|\underbrace{a|n\rangle}_{\sqrt{n}|n-1\rangle} = \sqrt{n}\,\delta_{n',n-1}$ $\quad \langle n'|a^+|n\rangle = \sqrt{n+1}\,\delta_{n',n+1}$

$$\begin{array}{c|c} & n \\ \hline n' & a = \begin{pmatrix} 0 & \sqrt{1} & & & 0 \\ & 0 & \sqrt{2} & & \\ & & 0 & \sqrt{3} & \\ & & & 0 & \ddots \\ 0 & & & & \ddots \end{pmatrix}\end{array} \qquad a^+ = \begin{pmatrix} 0 & & & & 0 \\ \sqrt{1} & 0 & & & \\ & \sqrt{2} & 0 & & \\ & & \sqrt{3} & 0 & \\ 0 & & & \ddots & \ddots \end{pmatrix}$$

E-repr.

oper $\hat{x} \longleftrightarrow \underbrace{\langle n' | \hat{x} | n \rangle}$ $= \frac{x_0}{\sqrt{2}} \begin{pmatrix} 0 & \sqrt{1} & & & \\ \sqrt{1} & 0 & \sqrt{2} & & 0 \\ & \sqrt{2} & 0 & \sqrt{3} & \\ & & \sqrt{3} & \ddots & \ddots \\ 0 & & & \ddots & \ddots \end{pmatrix}$ $p = \frac{i\hbar}{\sqrt{2} x_0} \begin{pmatrix} 0 & -\sqrt{1} & \cdot \\ +\sqrt{1} & 0 & -\sqrt{2} \\ & +\sqrt{2} & 0 \\ & & \ddots \end{pmatrix}$

Dodatek – vlastnosti oscilátorové báze $\{|n\rangle\}$

$\langle x | n \rangle \equiv \phi_n(x)$ ... Formanek, Cohen-Tannoudji

$\phi_0(q) \longleftrightarrow x$ $\boxed{\phi_0(x) = \frac{1}{\sqrt{x_0 \sqrt{\pi}}} e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2}}$

$x = x_0 q$

$x_0 \int dq$ $a^+ = \frac{1}{\sqrt{2}}\left(q - \frac{d}{dq}\right)$

$\phi_n(q)$ ... $\frac{(a^+)^n}{\sqrt{n!}}$ ... $\longrightarrow \phi_n(q) = \frac{(a^+)^n}{\sqrt{n!}} \phi_0(q)$

$$\phi_n(q) = \frac{1}{\sqrt{\sqrt{\pi}\; 2^n n!}} \underbrace{\left[q - \frac{d}{dq}\right]^n e^{-\frac{1}{2}q^2}}$$

$dq \to dx$

$$\phi_n(q) = \frac{1}{\sqrt{\sqrt{\pi}\; 2^n n!}} H_n(q)\, e^{-\frac{1}{2}q^2}$$

kde $H_n(q) \equiv e^{\frac{1}{2}q^2} \left[q - \frac{d}{dq}\right]^n e^{-\frac{1}{2}q^2}$

Hermiteovy polynomy

$$\phi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\, x_0\, 2^n n!}} H_n\left(\frac{x}{x_0}\right) e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2} \longleftarrow$$

pozn.
OBECNĚ o OG polynomech. $\{P_0(x), P_1(x), \ldots\}$

$(P_n, P_{n'})_w \equiv \int_\Omega P_n(x) P_{n'}(x)\, w(x)\, dx \overset{st.}{=} A_n \delta_{nn'}$

$w(x)$ – funkce $w(x) \geq 0$

Gram-Schmidt $\{1, x, x^2, x^3, \ldots\} \to \{P_0, P_1, P_2 \ldots\}$

pro nás ... $\{H_0(q), H_1(q), H_2(q), \dots\}$ OG poly

$w = e^{-q^2}$ $\mathcal{I} = \mathbb{R}$ $\longrightarrow$ Hermite

obecně OG poly ... $x P_n = a P_{n+1} + b P_n + c P_{n-1}$

Hermite $\langle x|\hat{X}|n\rangle = x\,\phi_n(x) = \frac{x_0}{\sqrt{2}}\left(\langle x|a|n\rangle + \langle x|a^\dagger|n\rangle\right)$

$\hat{X} = \frac{a+a^\dagger}{\sqrt{2}}$; $\langle x|$: x-reprez. ; $|n\rangle$: $\phi_n(x)$; $\sqrt{n}$, $\sqrt{n+1}$

$$= \frac{x_0}{\sqrt{2}}\left(\sqrt{n}\,\phi_{n-1}(x) + \sqrt{n+1}\,\phi_{n+1}\right)$$

$$\phi_{n+1} = f(\phi_n, \phi_{n-1})$$

$$\boxed{\frac{x}{x_0} H_n\left(\frac{x}{x_0}\right) = n H_{n-1}\left(\frac{x}{x_0}\right) + \frac{1}{2} H_{n+1}\left(\frac{x}{x_0}\right)}$$

$H_0 = 1$
$H_{-1} = 0$

Rekurentní relace

- vytvářející funkce: $f(x,t) = \exp\{2xt - t^2\}$

$$\boxed{f(x,t) = \sum_{n=0}^{\infty} \frac{1}{n!} H_n(x)\, t^n}$$

H_n

$\langle n|x|n'\rangle$

$$H_n(x) = \frac{d^n}{dt^n} f(x,t)\Big|_{t=0}$$

POZNÁMKA: stacionární stavy LHO

-- hledání řešením ODR $\hat{H}\psi(x) = E\psi(x)$