# Kvantna mehanika

## Schrödingerjeva enačba

Dejstva: i) $E = \hbar\omega = h\nu \; ; \; \hbar = \frac{h}{2\pi}$ (Bohr, Einstein)

ii) $p = \hbar k \; ; \; k = \frac{2\pi}{\lambda}$ (de Broglie)

iii) $E = \frac{p^2}{2m}$

iv) Vsak skupaj je mehanično valovanje

Kakšne enačbe že poznamo (v tistem času)?

a) Valovna enačba $$\frac{\partial^2 u}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} \; ; \; u = u_0 \cos(kx - \omega t)$$

vstavi nastavek

$$-k^2 = -\frac{\omega^2}{c^2} \Rightarrow \underset{E}{\omega} = \pm c\,|\underset{p}{k}| \qquad E \propto p \quad X$$

Ne bo ok

b) Difuzijska enačba $$D\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t} \; ; \; T = T_0 \cos kx \cos\omega t$$

Stoječi val

$$-k^2 D\, T(x,t) = -\omega T_0 \sin\omega t \cos kx \;\; \not\propto T(x,t)$$

Vzamemo raje nastavek: $T = T_0 e^{i(kx - \omega t)}$ in dobimo

$$\underset{p^2}{k^2} D = i\underset{E}{\omega} \; ; \; \omega, k \in \mathbb{R} \quad D = ? \in \mathbb{C}$$

Res sorazmerno s kvadratom?

$$D = \frac{i\omega}{k^2} = \frac{i\hbar^2 k^2}{\hbar\, 2mk^2} = i\frac{\hbar}{2m} \Rightarrow E = \frac{p^2}{2m}$$

✓ To pa ok!

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \qquad \psi = \psi_0 e^{i(kx-\omega t)}$$

To velja za prost delec!

Dodamo torej še potencial če delec ni prost:

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

## Kaj je $\psi$?

$\psi = \alpha + i\beta \quad ; \; \alpha, \beta \in \mathbb{R}$ Ta nastavek z Re in Im delom vstavimo v schrodingerjevo enačbe

$$i\hbar(\dot{\alpha} + i\dot{\beta}) = -\frac{\hbar^2}{2m}(\alpha'' + i\beta'') + V(\alpha + i\beta)$$

Potiho privzamemo da je V realen

$$\left.\begin{aligned} -\hbar\dot{\beta} &= -\frac{\hbar^2}{2m}\alpha'' + V\alpha \\ \hbar\dot{\alpha} &= -\frac{\hbar^2}{2m}\beta'' + V\beta \end{aligned}\right\}$$ 2 sklopljeni dif. en. $\in \mathbb{R}$

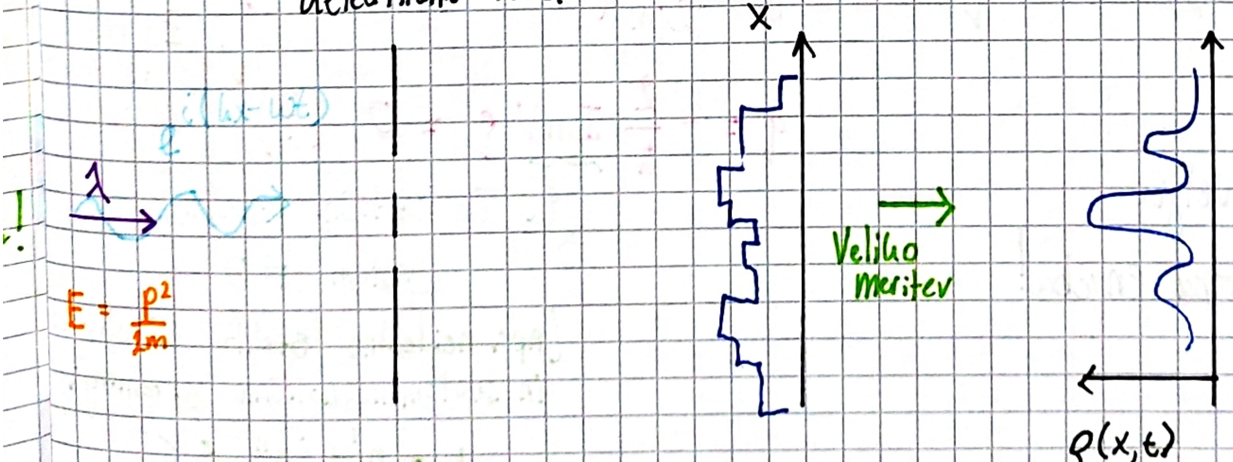
Max Born: $|\psi(\vec{r},t)|^2 = \rho(\vec{r},t)$ — $\psi^2$ je verjetnostna gostota za detekcijo delca v volumnu $dV$

$$dP(\vec{r},t) = \rho \, dV$$

$\psi$ je "verjetnostna amplituda"

$$\rho(\vec{r},t) = |\psi(\vec{r},t)|^2 = \alpha^2(\vec{r},t) + \beta^2(\vec{r},t)$$

Kaj je $\vec{r}$? To <u>ni</u> koordinata delca. Vemo lahko le verjetnost da pri $\vec{r}$ detektiramo delec.




Ta enačba nič nima z delcem ampak z verjetnostjo izida eksperimenta.
Kvantna mehanika ne opisuje delcev direktno.

# Kontinuitetna enačba za Verjetnost

Delec je nekje.

Normalizacija

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

Verjetnost

Splošna kontinuitetna enačba: $\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = q$

Preverimo to kontinuitetno enačbo za našo gostoto:

$$\frac{\partial}{\partial t}|\psi|^2 = \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t}$$

Iz SE:

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

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

$$\Rightarrow \frac{\partial}{\partial t}|\psi|^2 = -\frac{\hbar^2}{2m(-i\hbar)}\left(\frac{\partial^2 \psi^*}{\partial x^2}\right)\psi + \frac{V^*}{-i\hbar}\psi^*\psi + c.c.$$

complex conjugate

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

$$\Rightarrow \frac{\partial}{\partial t}|\psi|^2 = -\frac{\partial}{\partial x}\left(\frac{\hbar}{2im}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right)\right) - \frac{2}{\hbar}\,\mathrm{Im}(V)\,|\psi|^2$$

Vidimo:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} j_x = q$$

$$\vec{j} = \frac{\hbar}{2im}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$$

$$q = -\frac{2}{\hbar}\,\mathrm{Im}V\,\rho = 0 \quad (?)$$

Za nas $V$ bo to vedno veljalo

↳ če optični potencial potem $\neq 0$

(npr. neidealno steklo ki absorbira in se lomni količnik spremeni $n = n' + in'' \in \mathbb{C}$ uporabimo kompleksni lomni količnik)

Torej velja kontinuitetna enačba!

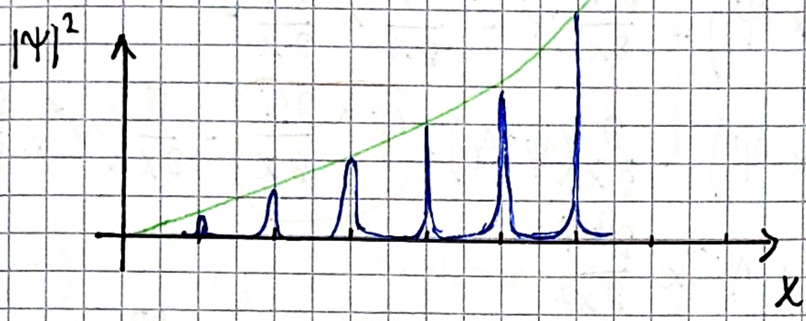
# Lastnosti Valovne funkcije

- $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$ ; $\psi \in \mathbb{C}$

Kako je pri $|x| \to \infty$?

Primer:

$\psi = Cx^2 e^{-x^2 \sin^2 x}$ $\qquad x_n = \pi n$ (ničla sinusa)




Ta se da normirati za $C < \infty$, tudi če ne gre proti 0 v $\pm\infty$

Tipično pa $\psi(x,t) \xrightarrow[|x|\to\infty]{} 0$, ker narava tako dela.

Ponavadi delamo v Schwartzovem prostoru (hitro padajočih funkcij)

$$\int_{-\infty}^{\infty} x^n |\psi|^2 dx = C < \infty$$

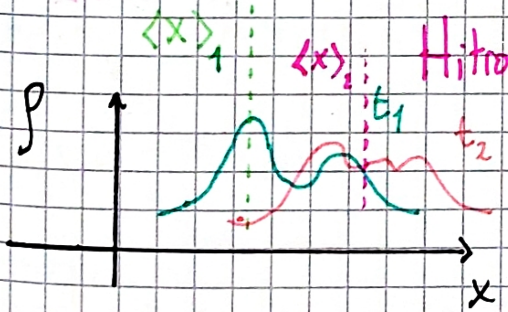
Hitreje padajo kot vsak polinom (Glej Mat 4)

Primeri:

- $\psi = f(x) e^{-\lambda x}$

$f(x) e^{-\lambda x^2}$

Hitrost težišča porazdelitve




Povprečna vrednost: $\overline{x}$

Pričakovana vrednost: $\langle x \rangle$

$$\langle x \rangle = \int x \rho \, dx = \int x \psi^*(x,t) \psi(x,t) dx = \int \psi^* x \psi \, dx$$

$$v_T = \frac{d}{dt}\langle x\rangle = \int_{-\infty}^{\infty}\left(\frac{\partial\psi^*}{\partial t}\, x\, \psi + \psi^* \underbrace{\frac{\partial x}{\partial t}}_{=0}\psi + \psi^* x \frac{\partial \psi}{\partial t}\right) dx =$$

Ker je $x$ neodvisna koordinata

Odvode spet iz Schrödingerjeve enačbe

$$= \frac{\hbar^2}{2mi\hbar}\int\left(\frac{\partial^2\psi^*}{\partial x^2}\, x\, \psi - c.c.\right) dx = (*)$$

Spravimo na [illegible]

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

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

$$\Rightarrow (*) = \frac{\hbar^2}{2i\hbar m}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\underbrace{\left(\frac{\partial\psi^*}{\partial x}x\psi - |\psi|^2 - \psi^* x \frac{\partial\psi}{\partial x}\right)}_{\text{Gre proti 0 v } \pm\infty} dx + \frac{1}{m}\int_{-\infty}^{\infty}\psi^*\left(-i\hbar\frac{\partial}{\partial x}\psi\right)dx =$$

Tako dobimo:

$$m\frac{d\langle x\rangle}{dt} = \int \psi^* \hat{p}\, \psi\, dx \, ;$$

Pričakovana vrednost operatorja gibalne količine

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

$$\hat{\vec{p}} = -i\hbar\nabla$$

Operator gibalne količine

(To ni od delca [illegible] ampak [illegible] pa to rečeno).

$$\boxed{\langle\hat{p}\rangle = m\frac{d\langle\hat{x}\rangle}{dt}}$$

# Operatorji

Operator deluje na funkcije

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

$$\hat{p}^2 = \hat{p}\hat{p} = -i\hbar \frac{\partial}{\partial x}\left(-i\hbar \frac{\partial}{\partial x}\right) = (-i\hbar)^2 \frac{\partial^2}{\partial x^2}$$

$$\hat{p}^n = (-i\hbar)^n \frac{\partial^n}{\partial x^n}$$

$\hat{x}$

$\hat{\vec{r}} = (\hat{x}, \hat{y}, \hat{z}) = (x, y, z)$

$\hat{V} = V(x,t)$

$$\boxed{\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}}$$

Hamiltonov operator

$f(z) = \sum_n c_n z^n$ analitična funkcija

Definiramo funkcijo operatorja kot: $f(\hat{A}) = \sum_n c_n \hat{A} z^n$

npr. $e^{\hat{A}} = 1 + \hat{A} + \frac{1}{2!}\hat{A}^2 + \ldots + \frac{1}{n!}\hat{A}^n + \ldots$

Identiteta

$1\Psi = \Psi$; $1 = I = \mathbb{1}$

## Komutatorji

Operatorji $\hat{A}, \hat{B}, \hat{C}, \ldots$

definiramo komutator med $\hat{A}$ in $\hat{B}$ kot: $\boxed{[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}}$

Lastnosti:

- $[\lambda \hat{A}, \hat{B}] = \lambda[\hat{A}, \hat{B}]$; $\lambda \in \mathbb{C}$
- $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$
- $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$

Dokaz: $= \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B} + \hat{A}\hat{C}\hat{B} - \hat{C}\hat{A}\hat{B} = [\hat{A}\hat{B}, \hat{C}]$

$\therefore$ $[\hat{A},[\hat{B},\hat{C}]] + [\hat{B},[\hat{C},\hat{A}]] + [\hat{C},[\hat{A},\hat{B}]] = 0$ Jacobijeva

$\therefore$ Baker-Hausdorffova lema

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}] + \frac{1}{2!}[\hat{A},[\hat{A},\hat{B}]] + \dots + \frac{1}{n!}\underbrace{[\hat{A},[\hat{A},[\dots}_{n\ \hat{A}},\hat{B}]\dots] + \dots$$

Primer:

$\hat{A} = \hat{x}$

$\hat{B} = \hat{p} = -i\hbar\frac{\partial}{\partial x}$

$$[\hat{x},\hat{p}] = ?$$

Poissonovi oklepaji

$\{p,q\} = \dots = 1$

Vzamemo splošno funkcijo $f(x)$ in poglejmo kaj naredi operator:

$$[\hat{x},\hat{p}]f(x) = x\left(-i\hbar\frac{\partial}{\partial x}\right)f + (i\hbar)\frac{\partial}{\partial x}(xf) =$$

$$= -i\hbar x\frac{\partial f}{\partial x} + i\hbar f + i\hbar x\frac{\partial f}{\partial x} = -i\hbar f$$

$[\hat{p},\hat{x}] = -i\hbar$ $\qquad$ $[\hat{x}_\alpha,\hat{p}_\beta] = i\hbar\delta_{\alpha\beta}$

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

V 3D:

$\hat{A} = \vec{r}$

$\hat{B} = \vec{p}$

$$[p_\alpha, r_\beta] = i\hbar\delta_{\alpha,\beta}$$

Podobno kot pri Poissonovih:

$\{p_\alpha, q_\beta\} = \delta_{\alpha\beta}$

# Lastnosti $p$ in $H$

Per partes: $\int u\,dv = uv - \int v\,du$

Naj bosta $f$ in $\psi$ poljubni funkciji:

Naprej res če gresta funkciji proti nič v $\pm\infty$, kar je ok za valovne funkcije

1.) $$\int_{-\infty}^{\infty} f\frac{\partial}{\partial x}\psi\,dx = f\psi\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\psi\frac{\partial f}{\partial x}\,dx = 0 - \int_{-\infty}^{\infty}\left(\frac{\partial f}{\partial x}\right)\psi\,dx$$

Operator $\hat{A} = \frac{\partial}{\partial x}$ je anti-simetričen / anti-hermitski

2.) $$\int_{-\infty}^{\infty} f \frac{\partial^2}{\partial x^2}\psi \, dx = -\int_{-\infty}^{\infty} \frac{\partial f}{\partial x}\frac{\partial \psi}{\partial x} dx = \int_{-\infty}^{\infty} \frac{\partial^2 f}{\partial x^2}\psi \, dx$$

Spet isti pogoj o padanju

Operator $\hat{A} = \frac{\partial^2}{\partial x^2}$ je simetričen/hermitski

3.) $\hat{A} = \hat{p} = -i\hbar \frac{\partial}{\partial x}$

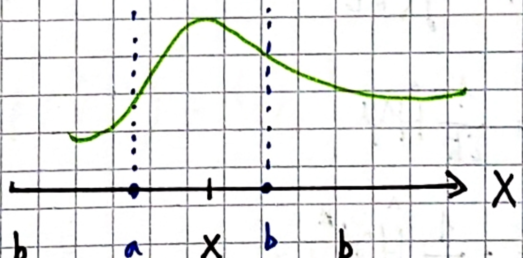
$$\int_{-\infty}^{\infty} f^* \hat{A}\psi \, dx = \int_{-\infty}^{\infty} f^*\left(-i\hbar\frac{\partial}{\partial x}\psi\right) dx = -\int_{-\infty}^{\infty} \left(\frac{\partial f^*}{\partial x}\right)(-i\hbar\psi)\, dx =$$

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

Torej je operator gibalne količine simetričen/hermitski

$$\int f^*\hat{A}\psi \, dx = \int (\hat{A}f)^*\psi \, dx$$

Intermezzo: Lastnosti $\psi$




1) $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$

2) $\psi$ je zvezna

3) $$i\hbar\frac{\partial}{\partial t}\int_a^b \psi \, dx = -\frac{\hbar^2}{2m}\int_a^b \frac{\partial^2 x}{\partial x^2} dy + \int_a^b V\psi \, dx$$

3) $\frac{\partial \psi}{\partial x} = ?$

Ko gre $\underline{b \to a}$:

$$i\hbar\frac{\partial \psi}{\partial t}(b-a) = -\frac{\hbar^2}{2m}\left(\frac{\partial \psi}{\partial x}\Big|_b - \frac{\partial \psi}{\partial x}\Big|_a\right) + \psi\int_a^b V \, dx$$

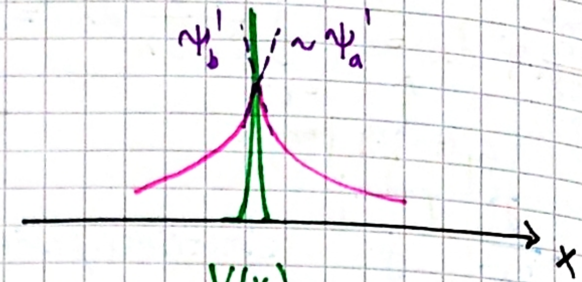
$b \to a$

$$0 = -\frac{\hbar^2}{2m}\left(\psi'(b) - \psi'(a)\right) + \psi\int_a^b V \, dx$$

a) $V$ zvezen $\equiv 0 \Rightarrow \psi'$ zvezna

b) $\psi'$ ima skok če je $V \propto \delta$

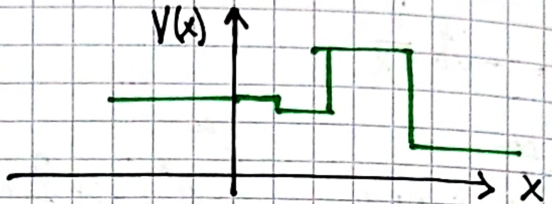
$$V(x) \sim \lambda \delta(x)$$




4) $\psi'' = ?$

Če ima $V$ skok v točki $x$,

ga ima tudi $\psi''$.




# Erhenfestov teorem (1927)

$i\hbar \frac{\partial \psi}{\partial t} = H\psi$

Imamo $\hat{A}, \psi$ in računamo $\langle \hat{A} \rangle$. Zanima nas:

$d^3r$ v 3D

$$\langle \hat{A} \rangle = \int \psi^* \hat{A} \psi \, dx$$

$\hat{A} = x$

$\hat{A} = \hat{p}$

$\hat{A} = V(\vec{r}, t)$

$\hat{A} = \hat{O} e^{i\omega t}$ ...

$$\frac{d}{dt}\langle \hat{A} \rangle = \int \left( \frac{\partial \psi^*}{\partial t} \hat{A} \psi + \psi^* \frac{\partial \hat{A}}{\partial t} \psi + \psi^* \hat{A} \frac{\partial \psi}{\partial t} \right) dx =$$

Od zadnjič:

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} \hat{H} \psi$$

$$\frac{\partial \psi^*}{\partial t} = -\frac{1}{i\hbar} \hat{H} \psi^*$$

Zadnjič gledali $a \to 0$ ko $|x| \to \infty$. To je ključno tu. $\hat{H}$ ni hermitski če to ne bi veljalo.

$\hat{H}$ lahko deluje na levo ali pa desno (hermitski op.)

Torej:

$$\frac{d}{dt}\langle \hat{A} \rangle = \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{1}{i\hbar} \int \left( (-\hat{H}\psi)^* \hat{A} \psi + \psi^* \hat{A} \hat{H} \psi \right) dx =$$

Komutator

$$= \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{1}{i\hbar} \int \left( \psi^* \hat{A} \hat{H} \psi - \psi^* \hat{H} \hat{A} \psi \right) dx =$$

Kot pri Klm:

$\frac{df}{dt} = \frac{\partial f}{\partial t} + \{f, H\}$ če $f(p,q)$

$$\Rightarrow \quad \frac{d}{dt}\langle \hat{A} \rangle = \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{1}{i\hbar} \left\langle [\hat{A}, \hat{H}] \right\rangle$$

## Primeri:

a) $\hat{A} = \hat{X} = x$

$$\frac{d\langle x\rangle}{dt} = 0 + \frac{1}{i\hbar}\left\langle \left[x, \frac{\hat{p}^2}{2m} + V(x,t)\right]\right\rangle = ?$$

Potrebujemo:

$$[x, \hat{p}^2] = \hat{p}\underbrace{[x,\hat{p}]}_{i\hbar} + \underbrace{[x,\hat{p}]}_{i\hbar}\hat{p} = 2i\hbar\hat{p}$$

$$[x, V] = 0$$

$$\frac{d\langle x\rangle}{dt} = \frac{1}{i\hbar}\frac{1}{2m}2i\hbar\langle\hat{p}\rangle = \frac{1}{m}\langle\hat{p}\rangle$$

b) $$\frac{d\langle\hat{p}\rangle}{dt} = m\frac{d^2\langle x\rangle}{dt^2} = 0 + \frac{1}{i\hbar}\langle[\hat{p},\hat{H}]\rangle = \frac{1}{i\hbar}\left\langle\left[\hat{p}, \frac{\hat{p}^2}{2m} + V\right]\right\rangle =$$

$$= \frac{1}{i\hbar}\left(\underbrace{\left\langle\left[\hat{p}, \frac{\hat{p}^2}{2m}\right]\right\rangle}_{0} + \langle[\hat{p},\hat{V}]\rangle\right) = (*)$$

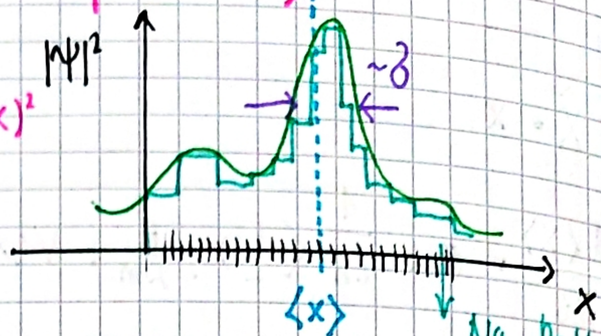
$$[\hat{p},\hat{V}]f = (pV - Vp)f = -i\hbar\frac{\partial}{\partial x}(Vf) + i\hbar V\frac{\partial}{\partial x}f =$$
$$= -i\hbar\left(\frac{\partial}{\partial x}V\right)f - i\hbar\left(\frac{\partial f}{\partial x}\right)V + i\hbar V\frac{\partial f}{\partial x} =$$
$$= -i\hbar\frac{\partial V}{\partial x}f \rightarrow \text{Za vsak } f$$

$$\Rightarrow (*) = \frac{1}{i\hbar}(-i\hbar)\left\langle\frac{\partial V}{\partial x}\right\rangle = -\left\langle\frac{\partial V}{\partial x}\right\rangle$$

Oz. v 3D: Erhenfestov teorem

$$m\frac{d^2\langle\vec{r}\rangle}{dt^2} = \langle\vec{F}(\vec{r},t)\rangle; \quad \vec{F}(\vec{r},t) = -\nabla V(\vec{r},t)$$

# Nedoločenost (širina porazdelitve)




$$\delta^2 = \langle x^2\rangle - \langle x\rangle^2 = \langle (x-\langle x\rangle)^2\rangle = (\Delta x)^2$$

$\uparrow$

Širina verjetnostne porazdelitve (ne da delec okol tega zmedeno frči, spet nič ne pove to o "delcu")

Na podlagi veliko diskretnih meritev lahko dobimo porazdelitev

To lahko naredimo tudi za operator $(\Delta\hat{A})^2 = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$, recimo Heisenberg je naredil $(\Delta p)^2 = \langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2$.


$$\Delta A \Delta B \geq \frac{1}{2}\left|\langle[\hat{A},\hat{B}]\rangle\right|$$

Tako dobimo Heisenbergov princip nedoločenosti:

$$\underline{\Delta x \Delta p_x \geq \frac{\hbar}{2}}$$ Relacija nedoločenosti

Če bi merili $p$, $\langle p\rangle$, $\Delta p$ in potem za drug delec $x$, $\langle x\rangle$, $\Delta x$ (v isti VF) bi za produkt to veljalo. To nič nima, da "delec" nima definirane lege in hitrosti. Govori o širinah porazdelitev.

# Formalizem Kvantne Mehanike

- Dirac (relativistična oblika SE)
- von Neumann (pripeljal funkcionalno analizo iz matematike v QM)

## 1. Vektorski prostor; Hilbertov prostor $L^2$

$$\Psi(\vec{r}, t) \in L^2$$

$\exists$ baza $\{f_n\}$; $n \in \mathbb{N}_0$ (števna baza)

(možno tudi $\{f_k\}$; $k \in \mathbb{R}$ ampak to je potem Banachov in ne Hilbertov prostor).

## 2. Skalarni produkt

$$(f, \Psi) = (f|\Psi) = \langle f, \Psi \rangle = \langle f | \Psi \rangle = \int_{-\infty}^{\infty} f^* \Psi \, dx$$

fiziki

$z \to z^*$ fiziki

$z \to \bar{z}$ matematiki

Lastnosti:

- $\langle f | \Psi \rangle = \langle \Psi | f \rangle^*$
- $\langle \Psi | \Psi \rangle \geq 0$, če $\langle \Psi | \Psi \rangle = 0 \Leftrightarrow \Psi = 0$
- $|\langle f | \Psi \rangle|^2 \leq \langle f | f \rangle \langle \Psi | \Psi \rangle$

## 3. Ket (iz bracket)

$\Psi(x, t) \in L^2$

Lahko rečemo, da stanje opišemo z vektorjem v Hilbertovem prostoru $L^2$ (ne govorimo, da je to enako psi)

$$|\Psi\rangle \in L^2$$

## 4. Linearni Operatorji:

$$\hat{A}\Psi = \Psi_1$$

$\mathcal{D}(\hat{A})$ domena operatorja (na katerih funkcijah dela)

Za linearne operatorje mora veljati:

$$\hat{A}(\lambda\Psi + \mu f) = \lambda\hat{A}\Psi + \mu\hat{A}f \,; \; \lambda, \mu \in \mathbb{C}$$

## 5. bra; $\langle bra | ket \rangle$

Spomnemo se linearnega funkcionala, ki funkcijo oz. vektor preslika v število.

$\psi(x) \in L^2$ $\hat{f}\psi = z$ $z \in \mathbb{C}$

Rieszov (reprezentacijski) izrek:

$$\forall \hat{f}\psi = z \Rightarrow \exists f_z \in L^2 :$$

$$z = \int f_z^*(x)\psi(x)\,dx = \langle f_z | \psi \rangle$$

$$\hat{f} \dashrightarrow \langle f| \quad \text{bra}$$

$$\hat{f}\psi = \int f_z^*(x)\psi(x)\,dx$$

$$\hat{f}\underset{\dots}{\overset{\psi}{\downarrow}} = \int f_z^*(x) \underset{\dots}{\overset{\psi}{\downarrow}}\,dx$$

$$\langle f| \dots |\psi\rangle \to \langle f||\psi\rangle = \langle f|\psi\rangle \in \mathbb{C}.$$

Operator, ki iz funkcije naredi število je funkcional.

## 6. Razvoj stanja po dani bazi

$\{f_n\}$ ortonormirana baza $\int f_n^* f_m\,dx = \delta_{n,m}$ (neskončno) števna

$$\psi(x) = \sum_n c_n f_n(x) \quad \text{razvoj po bazi}$$

Zaradi ortonormiranosti:

$$\int f_m^* \psi\,dx = \sum_n c_n \overset{\int f_n^* f_m\,dx}{\delta_{mn}} = \underline{\underline{c_m}}$$

$$\psi(x) = \sum_n \left( \int_{-\infty}^{\infty} \varphi_n^*\ \dots\ dx' \right) \varphi_n(x) \psi(x) \qquad I = \sum_n \varphi_n \int \varphi_n^*(x') \dots dx'$$

Ponovimo to "po Diracu":

$$\{|\varphi_n\rangle\} = \{|n\rangle\} \rightarrow |\varphi_n\rangle = |n\rangle$$

$$|\psi\rangle = \sum_n c_n |n\rangle \quad \Big/ \cdot \langle m|$$

$$\langle m|\psi\rangle = \sum_n c_n \underbrace{\langle m|n\rangle}_{\delta_{m,n}} = c_m$$

"$2\vec{a} = \vec{a}\, 2$
$2\psi = \psi\, 2$"

$$|\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle =$$

$$= \sum_n |n\rangle \langle n|\psi\rangle = \left( \sum_n |n\rangle\langle n| \right) |\psi\rangle =$$

$$= I\, |\psi\rangle ;$$

Identiteta "po Diracu"

$$\Rightarrow \quad I = \sum_n |n\rangle\langle n| \quad ; \quad I\psi = \psi$$

Paul Adrien Maurice Dirac intermezzo

Verjetno nekoliko avtistizen. Zelo je bil varčen pri notaciji. Ni se matematično preveč mučil.

John von Neumann intermezzo

Jud iz Madžarske, ki je emigriral v ameriko. Napisal knjigo, kjer je napisal formalizem / osnove glede na funkcionalno analizo.

# 7. Zapis operatorja v dani bazi

Matrični element

$$A_{mn} = \langle m|\hat{A}|n\rangle$$

$\{|n\rangle\}$ baza (ortonormirana)

$\hat{A}|\Psi\rangle = |\Psi_1\rangle$ dani operator

$$\hat{A}|\Psi\rangle = I\hat{A}I|\Psi\rangle = \sum_m |m\rangle\langle m|\hat{A}\sum_n |n\rangle\langle n|\Psi\rangle = \sum_{m,n}|m\rangle A_{mn}\langle n|\Psi\rangle$$

Vrinemo kompletni sistem

$$\hat{A} = \sum_{mn}|m\rangle A_{mn}\langle n|$$

Konkreten primer:

$$|\Psi\rangle = \sum_n c_n|n\rangle \; ; \; |\Psi_1\rangle = \sum_n d_n|n\rangle$$

$\sum_m\left(\sum_n A_{mn}c_n\right)|m\rangle$ Ubistvu

Zaradi ort. $\delta_{nk}$

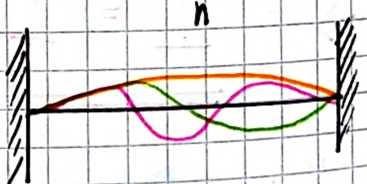
$$\hat{A}|\Psi\rangle = \sum_{mn}|m\rangle A_{mn}\underbrace{\langle n|\sum_k c_k|k\rangle}_{c_n} = \sum_{mn}|m\rangle A_{mn}c_n = \sum_m d_m|m\rangle = |\Psi_1\rangle$$

$$\Psi \rightarrow \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \\ \vdots \end{pmatrix} ; \; \hat{A}|\Psi\rangle = |\Psi_1\rangle$$

↳ To pomeni:

$$\begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_m \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & \cdots & \\ \vdots & & \ddots \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{pmatrix}$$

Primer: $\hat{A} = \hat{p} = -i\hbar\frac{\partial}{\partial x}$




$$\hat{p}\Psi(x) = -i\hbar\frac{\partial}{\partial x}\Psi(x) \; ; \; \mathcal{D}(\hat{p})$$

$$f_n(x) = C_n\sin(k_n x) \; ; \; |n\rangle$$

Matrične elemente dobimo:

$$\checkmark\, A_{mn} = \int_a^b C_m^* C_n \sin k_n x\left(-i\hbar\frac{\partial}{\partial x}\sin k_n x\right)dx$$

Funkcijo razvijemo po bazi:

$$\Psi = \sum_n c_n f_n \; ; \; c_n = \int f_n^*\Psi\,dx \Rightarrow c_n \checkmark$$

In takoj lahko delujemo z operatorjem na razvito funkcijo

$$d_m = \sum_m A_{mn} c_n$$

## 8. Hermitski ali simetrični operatorji

$$\langle f | \hat{A} | \psi \rangle = \langle f | \hat{A} \psi \rangle = \langle \hat{A} f | \psi \rangle$$ Simetričnost/Hermitskost

Lastnosti simetričnih operatorjev: (Od tu dalje operator $\hat{A} \to A$ (brez strešice) če je očitno, kaj je operator)

- Problem lastnih vrednosti

$$A|\psi\rangle = a|\psi\rangle \; ; \text{ isto ali pa } |\psi_a\rangle \text{ tudi isto}$$

$$A|a\rangle = a|a\rangle \quad / \cdot \langle \psi|$$

$$\langle \psi | A | \psi \rangle = a \langle \psi | \psi \rangle$$

Iz simetričnosti sledi

$$\langle A\psi | \psi \rangle = \langle \psi | A \psi \rangle = \langle \psi | A | \psi \rangle = a \underbrace{\langle \psi | \psi \rangle}_{\in \mathbb{R}} \in \mathbb{R}$$

$$\text{"} \langle \psi | A \psi \rangle^* = \langle \psi | A | \psi \rangle^* \qquad \Rightarrow a \in \mathbb{R}$$

Torej: Če je $\hat{A}$ simetričen ima vse lastne vrednosti realne.

- ..

$$A|\psi\rangle = a|\psi\rangle \; / \cdot \langle f| \quad \to \quad \langle f | A | \psi \rangle = a \langle f | \psi \rangle \; / \text{ nič ne naredimo}$$

$$A|f\rangle = b|f\rangle \; / \cdot \langle \psi| \qquad \langle \psi | A | f \rangle = b \langle \psi | f \rangle \; / \text{ kompleksno konjugiramo}$$

$$\to \quad \langle f | A | \psi \rangle = a \langle f | \psi \rangle \quad (1)$$

$$\langle \psi | A | f \rangle^* = b \langle f | \psi \rangle$$

$$\langle \psi | A | f \rangle^* = \langle \psi | A f \rangle^* = \langle A f | \psi \rangle \overset{\text{Simetričnost}}{=} \langle f | A \psi \rangle = \langle f | A | \psi \rangle$$

Še sklop dela take stvari

$$\Rightarrow \langle f | A | \psi \rangle = b \langle f | \psi \rangle \quad (2)$$

(1)-(2): $0 = (a-b) \langle f | \psi \rangle \Rightarrow$ če $a \neq b$ $\langle f | \psi \rangle = 0$

Torej: Lastni vektorji so med seboj ortogonalni

DN:

$$\langle f|A|\psi\rangle = \langle Af|\psi\rangle \Rightarrow \langle\psi|A|\psi\rangle \in \mathbb{R}$$

Dokaži da če so vse lastne vrednosti realne je operator hermitski (torej v drugo smer)

$$\exists|\psi\rangle : \langle\psi|A|\psi\rangle \in \mathbb{R} \Rightarrow \exists f,\psi \quad \langle f|A\psi\rangle = \langle Af|\psi\rangle$$

## 9. Hermitsko adjungirani operator

$$A;\ |f\rangle, |\psi\rangle$$

$$B: \langle f|A\psi\rangle = \langle Bf|\psi\rangle$$ Enak na levi kot A na desni.

$$B = A^\dagger$$ A dagger/bodalo `$A^\dagger$`

Matematika: $A \to A^*$ za $A^\dagger$ in $A \to \bar{A}$ za $A^*$

**Lastnosti:** (B tu nima iste vloge)

- $A = zB$

$$\langle f|A|\psi\rangle = \langle f|zB|\psi\rangle = z\langle f|B|\psi\rangle = z\langle B^\dagger f|\psi\rangle = \langle\psi|B^\dagger|f\rangle^*$$

$$\langle A^\dagger f|\psi\rangle = \langle z^* B^\dagger f|\psi\rangle$$

$$\Rightarrow \langle A^\dagger f|\psi\rangle = \langle z^* B^\dagger f|\psi\rangle$$

$$A = zI$$
$$A^\dagger = z^* I$$

Primer: $A = x \Rightarrow A^\dagger = x$

- $A = |m\rangle\langle n|$

$$\langle f|A|\psi\rangle = \langle f|m\rangle\langle n|\psi\rangle = \left(\langle\psi|n\rangle\langle m|f\rangle\right)^* = \langle A^\dagger f|\psi\rangle$$

$$\Rightarrow A^\dagger = |n\rangle\langle m| \quad A = |m\rangle\langle n|$$

- $(\mu A + \lambda B)^\dagger = \mu^* A^\dagger + \lambda^* B^\dagger$

:: $(AB)^\dagger$

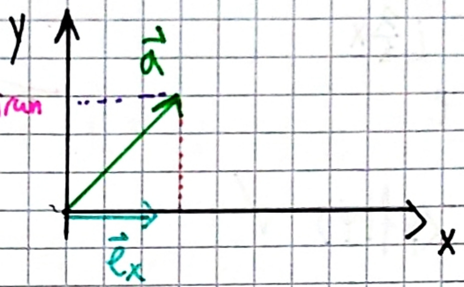
$$\langle f|AB|\psi\rangle = \langle A^\dagger f|B\psi\rangle = \langle B^\dagger A^\dagger f|\psi\rangle$$

$$\Rightarrow (AB)^\dagger = B^\dagger A^\dagger$$

:: Projektor

Sam sebi adjungiran

$$P_n = |n\rangle\langle n| = P_n^\dagger$$




Idempotentni operatorji:

$$P_n^2 = P_n P_n = |n\rangle\underbrace{\langle n|n\rangle}_{1}\langle n| = P_n$$

$$\vec{a} = (\vec{e}_x \cdot \vec{a})\vec{e}_x + (\vec{e}_y \cdot \vec{a})\vec{e}_y$$

$$P_x\vec{a} = (\vec{e}_x \cdot \vec{a})e_x \qquad P_y = (\vec{e}_y \cdots)\vec{e}_y$$

$$I = \sum_n P_n$$

10. Kako najdemo $A^\dagger$, če poznamo $A$?

$$\hat{A} = \sum_{mn} |m\rangle A_{mn}\langle n| \qquad (\hat{A})_{mn} = A_{mn}$$

Da je lepše $n \to m$ $m \to n$

$$A^\dagger = \sum_{mn} |n\rangle A^*_{mn}\langle m| = \sum_{mn} |m\rangle A^*_{nm}\langle n| \qquad (\hat{A}^\dagger)_{mn} = A^*_{nm}$$

Transponiranje in konjugiranje

11. Sebi adjungirani operatorji (... hermitski)

V fiziki nismo natančni kar se tiče imenovanja hermitski/sebi adjungirani.

Naj velja:

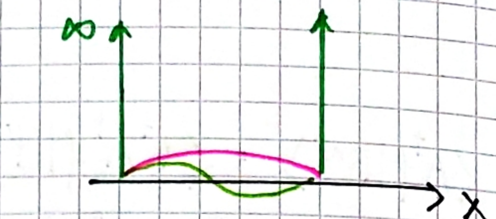
a) $\langle f|A|\psi\rangle = \langle Af|\psi\rangle$ hermitski simetričen

b) $A = A^\dagger$ → Mora veljati (a) in $\mathcal{D}(A) = \mathcal{D}(A^\dagger)$ (domena)

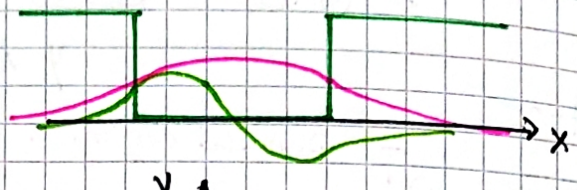
$$\Rightarrow \exists\{|n\rangle\};\ A|n\rangle = a_n|n\rangle$$

Primer/komentar:

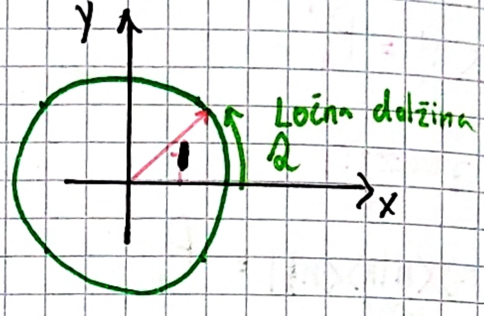
1) $\hat{A} = \hat{p} = -i\hbar \frac{\partial}{\partial x}$



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



$$\Rightarrow \quad f(x) = C e^{i\frac{\lambda}{\hbar}x}$$




a) $\langle f | \hat{p} \psi \rangle = \langle \hat{p} f | \psi \rangle$ ✓

$$f(0) = 0 \Rightarrow C e^{0} = C \Rightarrow \underline{\underline{C = 0}}$$

Torej ta operator ne dela baze, ker ni funkcij, da bi zadoščala robnim pogojem (domena funkcije, ki imajo na robu 0)

$$H = \frac{\hat{p}^2}{2m} \checkmark \qquad \hat{p} \to C_{\pm} e^{\pm i \frac{\lambda}{\hbar} x}$$

b) Periodični robni pogoji

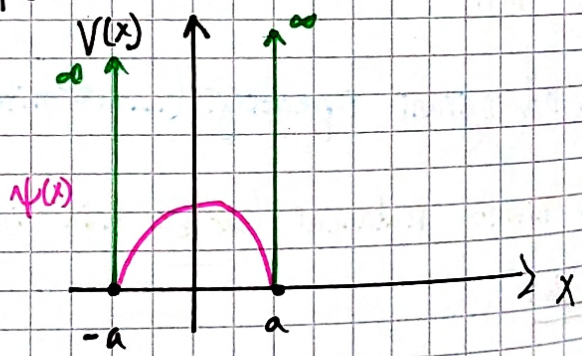
Pomembno, da sta domeni enaki!

$$f(\lambda + 2\pi) = f(\lambda)$$

$$C e^{i\frac{\lambda}{\hbar}(\lambda + 2\pi)} = C e^{i\frac{\lambda}{\hbar}\lambda} \; ; \; \lambda_n \in \mathbb{R}$$

2)

$$\psi(x) = C(a^2 - x^2)$$




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

Kaj so pričakovane vrednosti energije:

$$\langle H \rangle = \langle E \rangle = \int |C|^2 (a^2 - x^2)\left(-\frac{\hbar \partial^2}{2m \partial x^2}\right)(a^2 - x^2)\, dx \geq 0$$

Kolikšna je nedoločenost?

$$(\Delta E)^2 = \langle H^2 \rangle - \langle H \rangle^2$$

$$\langle H^2 \rangle = \int |C|^2 (a^2 - x^2)\left(\frac{\hbar^4}{(2m)^2}\frac{\partial^4}{\partial x^4}(a^2 - x^2)\right) dx = 0$$

$\Rightarrow \quad (\Delta E)^2 < 0 \quad (???)$ Patološki primer, ker to ne obstaja v naravi. DN da pogruntaj.

## 12. Unitarni operatorji

$U^{-1}$ ... inverzni operator $\quad U^{-1} = U^{\dagger}$ Unitaren operator!

$$U^{-1}U = UU^{-1} = I = U^{\dagger}U = UU^{\dagger}$$

Lastnosti:

- $\langle f|\psi\rangle$

$$U|f\rangle = |\tilde{f}\rangle \quad ; \quad |f\rangle = U^{-1}|\tilde{f}\rangle = U^{\dagger}|\tilde{f}\rangle$$
$$U|\psi\rangle = |\tilde{\psi}\rangle \quad ; \quad |\psi\rangle = U^{\dagger}|\tilde{\psi}\rangle$$

$$\langle f|\psi\rangle = \langle U^{\dagger}\tilde{f}|U^{\dagger}\tilde{\psi}\rangle = \langle \tilde{f}|\underbrace{UU^{\dagger}}_{I}|\tilde{\psi}\rangle = \langle \tilde{f}|\tilde{\psi}\rangle$$

Unitarni operatorji ohranjajo skalarni produkt

- $$\langle f|A|\psi\rangle = \langle U^{\dagger}\tilde{f}|A|U^{\dagger}\tilde{\psi}\rangle = \langle \tilde{f}|UAU^{\dagger}|\tilde{\psi}\rangle = \langle \tilde{f}|\tilde{A}|\tilde{\psi}\rangle$$

Pravzaprav transformacija/zamenjava baze, kjer je

$$\tilde{A} = UAU^{\dagger}$$

- $A = \mu B + \lambda CD \quad / \, U \cdot U^{\dagger} \quad , \, I = U^{\dagger}U$

$$\tilde{A} = \mu\tilde{B} + \lambda\tilde{C}\tilde{D}$$

- Če velja $K = K^{\dagger} \Rightarrow U = e^{iK}$ Unitaren

To ni tako očitno ker $e^{A}e^{B} \neq e^{A+B}$ enakost samo če AB komutirata.

a) $$UU^{\dagger} = e^{iK}e^{-iK} = I$$

b) Enoparametrični unitarni operator

$$U(\alpha): \exists K = K^{\dagger}: U(\alpha) = e^{i\alpha K}$$

hermitski

# 13. Časovni razvoj kvantnega stanja

- Stacionarna stanja ; $H \neq H(t)$

$$H = \frac{p^2}{2m} + V(\vec{r}) \qquad i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \; ; \quad \Psi(\vec{r},t) = \psi(\vec{r}) f(t)$$

$$\Rightarrow \quad i\hbar \psi(\vec{r}) \frac{\partial f}{\partial t} = H\psi f \, / : \psi f$$

$$i\hbar \left(\frac{df}{dt}\right) \frac{1}{f} = \frac{1}{\psi} H \psi = E \quad \text{konst.}$$

funkciji $t$ in $x$ $\Rightarrow$ strani sta konst.

Tvorijo bazo

$$\Rightarrow \quad \Psi(\vec{r},t) = \psi(\vec{r}) e^{-i\frac{E}{\hbar}t} \; ; \quad H\psi_n(\vec{r}) = E_n \psi_n(\vec{r})$$

$$|\Psi|^2 = |\psi|^2$$

- •

$$H|f_n\rangle = E_n |f_n\rangle$$

$$|\psi(t)\rangle\Big|_0 = \sum_n |f_n\rangle\langle f_n|\psi(0)\rangle =$$

čisto el

$$= \sum_n \underbrace{\langle f_n|\psi(0)\rangle}_{c_n} |f_n\rangle \quad \rightarrow f_n(\vec{r})$$

Stacionarna stanja, ki se po prvi točki spreminjajo po času

$$|\psi(t)\rangle = \sum_n \langle f_n|\psi(0)\rangle e^{-\frac{iE_n}{\hbar}t} |f_n\rangle$$

$$\Psi(\vec{r},t) = \sum_n c_n e^{-\frac{iE_n}{\hbar}t} f_n(\vec{r})$$

$$\hat{f}(\hat{A}) = \sum_n c_n \hat{A}^n \; ; \quad f(z) = \sum_n c_n z^n \; ; \quad z \in \mathbb{C}$$

$$\hat{A}|n\rangle = a_n |n\rangle$$

$$\hat{f}(\hat{A})|\psi\rangle = \sum_n c_n f(a_n) \psi$$

$$e^{-i\frac{E_n}{\hbar}t} f_n(\vec{r}) = e^{-i\frac{\hat{H}t}{\hbar}} f_n(\vec{r})$$

$$\hookrightarrow I - \frac{iE_nt}{\hbar} + \frac{1}{2!}\left(\frac{iE_n}{\hbar}\right)^2 t^2 \pm \mathcal{O}(t^3)$$

$$\Psi(\vec{r},t) = e^{-\frac{iH}{\hbar}t} \underbrace{\sum_n c_n f_n(\vec{r})}_{\psi(\vec{r},0)}$$

$$\Rightarrow \Psi(\vec{r},t) = e^{\frac{-iHt}{\hbar}} \psi(\vec{r},0) \quad ; \quad \underbrace{U(t) = e^{-\frac{iH}{\hbar}t}}$$

Unitarni operator časovnega razvoja

Translacija v času:

$$U(t_2,t_1) = e^{-i\frac{H}{\hbar}(t_2-t_1)} \quad ; \; e^{iK} = U \text{ kjer je } K \text{ "generator"}$$

$$\Psi(\vec{r},t_2) = U(t_2,t_1)\Psi(\vec{r},t_1)$$

$$\delta\Psi(\vec{r},t) = \Psi(\vec{r},t+dt) - \Psi(\vec{r},t) = U_{t+dt,t}\Psi(\vec{r},t) =$$

$$= \left(1 - i\frac{H}{\hbar}dt + \mathcal{O}(dt^2)\right)\Psi(\vec{r},t) - \Psi(\vec{r},t)$$

$$\Rightarrow \frac{d\Psi(\vec{r},t)}{dt} = -i\frac{H}{\hbar}\Psi(\vec{r},t) \Rightarrow \underbrace{i\hbar\frac{\partial\Psi}{\partial t} = H\Psi}$$

Ravno stacionarna SE

Torej Schrödingerjevo enačbo lahko izpeljemo samo iz tega, da je časoven razvoj unitaren.

## 14. Reprezentacija p in X

Spomnimo se FT:

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

$$\tilde{f}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-ikx'} dx'$$

Vstavimo:

$$f(x) = \int_{-\infty}^{\infty} \underbrace{\frac{1}{2\pi} \int_{-\infty}^{\infty} f(x') e^{-ikx'+ikx} dx\, dk}_{\delta(x-x')} = \int_{-\infty}^{\infty} \delta(x-x') f(x') dx'$$

To je bila originalna uvedba delta funkcije

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk$$

Diracova funkcija delta (ki ni funkcija, sama po sebi ne obstaja)

- • Prosti delec $V(x) = 0$

$p = \hbar k$

$$i\hbar \frac{d}{dt} |\psi\rangle = \frac{\hat{p}^2}{2m} |\psi\rangle \quad ; \quad |\psi\rangle \to |f_p\rangle = |p\rangle$$

$$\hat{p} |f_p\rangle = p |f_p\rangle \quad ; \quad p \in \mathbb{R}$$

$$-i\hbar \frac{\partial}{\partial x} f_{p_0}(x) = p_0 f_{p_0}(x) \Rightarrow f_{p_0} = C e^{i \frac{p_0}{\hbar} x}$$

↳ Se ne da normirati

$$\int_{-\infty}^{\infty} f_{p_0}^*(x) f_p(x) dx = \delta(p - p_0) ; \text{ kjer mora biti } C = \frac{1}{\sqrt{2\pi\hbar}}$$

$$\Rightarrow f_{p_0} = \frac{1}{\sqrt{2\pi\hbar}} e^{i \frac{p_0}{\hbar} x} \quad ; \quad |p_0\rangle = |f_{p_0}\rangle$$

$$\langle f_{p_0} | f_p \rangle = \delta(p - p_0) \text{ oz. } \boxed{\langle p_0 | p \rangle = \delta(p - p_0) = \delta(p_0 - p)}$$

(Primer števne baze $\{|\psi_n\rangle\}$ ; $\langle n|m\rangle = \delta_{mn}$ )

$\tilde{\psi}(p)$ v neskončni

$$\psi(x) = 1 \cdot \int \tilde{\psi}(p) f_p(x)\, dp \;;$$

pri števni bazi je to analog $\sum_n c_n \psi_n$

$$\tilde{\psi}(p) = 1 \cdot \int \psi(x) f_p^*(x)\, dx$$

2π pospravljen v normalizacijsko konstanto $f_p$

Parsevalova enačba
$$\int |\psi|^2 dx = \int |\tilde{\psi}|^2 dp$$

Diskreten analog
$$\int |\psi|^2 dx = 1 = \sum_n |c_n|^2$$

$$\therefore \quad \hat{p}\psi(x) = -i\hbar \frac{\partial}{\partial x}\psi(x) = $$ ; Razvijemo po lastnih funkcijah $\tilde{\psi}$ je amplituda v razvoju

$$= \int \tilde{\psi}(p)\underbrace{\left(-i\hbar \frac{\partial}{\partial x} f_p(x)\right)}_{p f_p(x)} dp = \int \left(p\tilde{\psi}(p)\right) f_p(x)\, dp$$

Torej to pomeni:

$$\left(-i\hbar \frac{\partial}{\partial x}\right)^n \psi(x) = \hat{p}^n \psi(x) = p^n \tilde{\psi}(p)$$

Poglejmo še:

$x \cdot \exp$ je isto kot odvod $\rightarrow i\hbar\frac{\partial}{\partial p}$ hermitski zato lahko na pravo funkcijo

$$\hat{x}\psi(x) = x\psi(x) = \int \tilde{\psi}(p)\, x f_p(x)\, dp = \int \left(i\hbar \frac{\partial}{\partial p}\tilde{\psi}\right) f_p(x)\, dp$$

Torej to pomeni:

$$x^n \psi(x) \overset{FT}{\longleftrightarrow} \left(+i\hbar \frac{\partial}{\partial p}\right)^n \tilde{\psi}(p)$$

Torej se pri FT operatorja ravno "obrneta" (in še predznak)

$\therefore$ $$\hat{x}\psi_0(x) = x\psi_0(x) = x_0\psi_0(x)$$ Iščemo lastne funkcije $\hat{x}$

Enako

$$x\int \tilde{\psi}(p) f_p(x)\, dp = \int \left(i\hbar \frac{\partial}{\partial p}\tilde{\psi}_0(p)\right) f_p(x)\, dp$$

v p prost. $i\hbar\frac{\partial}{\partial p}$ izpeljimo malo prej

Torej mora veljati:

Ravno konjugirano za p

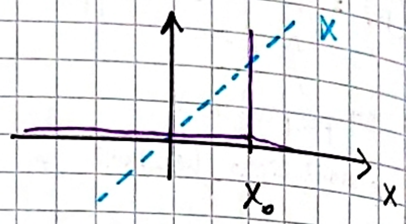
$$+i\hbar\frac{\partial}{\partial p}\tilde{\Psi}(p) = x_0\tilde{\Psi}(p) \Rightarrow \tilde{\Psi}_0(p) = \frac{1}{\sqrt{2\pi\hbar}}e^{-i\frac{p}{\hbar}x} = f_p(x)^*$$

FT lastne funkcije koordinate

To lahko transformiramo nazaj:

Lastne funkcije koordinate!

$$\Psi_0(x) = \int f_p(x_0)^* f_p(x)\,dp = \delta(x-x_0)$$




$$x\,\delta(x-x_0) = x_0\,\delta(x-x_0)$$

15. Verjetnostni amplitudi $\langle p|\Psi\rangle$ in $\langle x|\Psi\rangle$

$$\Psi(x) \in \mathbb{C}$$
$$\in L^2$$

Torej lahko gledamo na $\Psi$ kot vektor $\vec{\Psi}$ v $L^2$ ; $|\Psi\rangle \in L^2$

↑ Vsebuje info o izražavi v katerikoli bazi $\Psi(x), \tilde{\Psi}(p), \bar{\Psi}(u), c_n$

• $|\Psi\rangle = \int\tilde{\Psi}(p)|p\rangle\,dp \quad / \cdot\langle p_1|$

$$\langle p_1|\Psi\rangle = \int\tilde{\Psi}(p)\underbrace{\langle p_1|p\rangle}_{\delta(p-p_1)}dp = \int\tilde{\Psi}(p)\,\delta(p-p_1)\,dp = \tilde{\Psi}(p_1)$$

Amplituda

$$\Rightarrow \boxed{\tilde{\Psi}(p) = \langle p|\Psi\rangle} \in \mathbb{C}$$

•• Komentar: analog v števni bazi

$$|\Psi\rangle = \sum_n c_n|n\rangle \quad / \cdot\langle n_1|$$

$$\langle n_1|\Psi\rangle = c_{n_1} \Rightarrow c_n = \langle n|\Psi\rangle \in \mathbb{C}$$

∴ $|\Psi\rangle = \int\tilde{\Psi}(p)|p\rangle\,dp \quad / \cdot\langle x_0|$ ; $x|x_0\rangle = x_0|x_0\rangle$

$$\langle x_0|\Psi\rangle = \int\tilde{\Psi}(p)\underbrace{\langle x_0|p\rangle}_{f_p(x_0)}dp = \Psi(x_0)$$

$$\Rightarrow \boxed{\Psi(x) = \langle x|\Psi\rangle} \in \mathbb{C}$$

$$\hat{I} = \sum_n |n\rangle\langle n|$$

$$|\psi\rangle = \sum_n |n\rangle \underbrace{\langle n|\psi\rangle}_{c_n} = \sum_n c_n |n\rangle$$

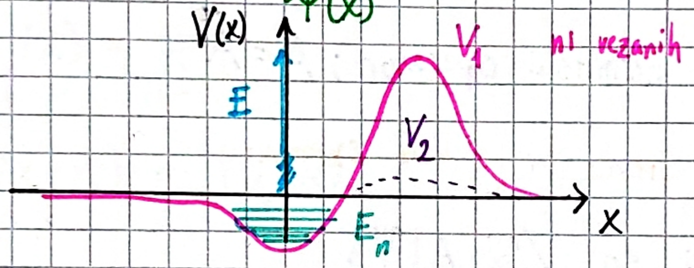
Lahko pa razvijemo tudi z integralom: $I = \int |p\rangle\langle p| dp$

$$|\psi\rangle = I|\psi\rangle = \int |p\rangle \underbrace{\langle p|\psi\rangle}_{\tilde{\psi}(p)} dp = \int \tilde{\psi}(p)|p\rangle dp$$

ali pa: $I = \int |x\rangle\langle x| dx$

$$|\psi\rangle = I|\psi\rangle = \int |x\rangle \underbrace{\langle x|\psi\rangle}_{\psi(x)} dx = \int \psi(x)|x\rangle dx$$

Primer




Integral potenciala mora biti negativen, da imamo vezana stanja (za 1D)

Za 3D mora biti "dovolj" negativen.

V splošnem imamo in vezana stanja in sipalna stanja.

$$I = \sum_n |E_n\rangle\langle E_n| + \sum_\nu \int |E,\nu\rangle\langle E,\nu| dE$$

16. Kompleten sistem med sabo komutirajočih operatorjev

Imamo A, B in komutirata $[A,B] = 0 \Leftrightarrow \exists \underbrace{\{|n\rangle\}}_{\text{baza}}$ : $A|n\rangle = a_n|n\rangle$, $B|n\rangle = b_n|n\rangle$

Primer: $\hat{H} = \frac{\hat{p}^2}{2m} = A$

$\hat{p} = B$

$\hat{L} = \hat{\vec{r}} \times \hat{\vec{p}} = C$

To velja tudi v drugo smer. Če najdemo bazo, ki je večim operatorjem lastna potem ti operatorji med sabo komutirajo.

Primer:

$$V(r) \propto \frac{1}{r} \quad ; \quad H, \vec{L}, L_z, \vec{S}, S_z, \vec{A}$$

Kvantni Laplace-Runge-Lenzov vektor

Ker ti operatorji med sabo komutirajo lahko stanje opišemo z njimi.

$$|\psi\rangle = |n, l, m_l, s, m_s\rangle$$

## 17. Postulati kvantne mehanike

mnogo drugih

- Kopenhagenska interpretacija (Bohr + ...)

bolj samo diskutiral

1. Svet razbijemo na kvantni in klasičen svet


$|\psi\rangle \in L^2$

2. Vsaka opazljivka je hermitski operator ; $A = A^\dagger$

↳ Vsako število, ki ga lahko izmerimo

3. Pričakovane vrednosti so $\langle \psi | A | \psi \rangle$

4. Dinamika (časovni razvoj)

Unitarno

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle \quad ; \quad |\psi(t)\rangle = U(t,0)|\psi(0)\rangle$$

5. O meritvi: Pri posamezni meritvi A je rezultat ena od lastnih vrednosti enačbe

a)

$$A|a\rangle = a|a\rangle \rightarrow a$$

Verjetnost, da izmerimo natanko „a" je podana z

$$P_a = |c_a|^2 \quad ; \quad c_a = \langle a | \psi \rangle$$

oz.

$$|\psi\rangle = \sum_n c_n |n\rangle \qquad |c_n|^2 = P_n \qquad |\psi\rangle = \int \psi(x)|x\rangle dx$$

$$|\psi(x)|^2 - \rho(x)$$

zvezne lastne vrednosti

b) Kolaps valovne funkcije: Po izvedeni meritvi je kvantni sistem v stanju $|a\rangle$

$$|\psi\rangle \xrightarrow{\text{kolaps}} |a\rangle \quad ; \quad \text{Neunitarno}$$

Razno / Ponovitev

$$\hat{p}|p_0\rangle = p_0|p_0\rangle \ ; \quad |\Psi\rangle$$

$$\hat{x}|x_0\rangle = x_0|x_0\rangle$$

$$|\Psi\rangle = \int |x\rangle \underbrace{\langle x|\Psi\rangle}_{\Psi(x)} dx = \int \Psi(x)|x\rangle dx \quad \rightsquigarrow |x_0\rangle ; \ x_0 ; \ |\Psi(x_0)|^2 dx = dP$$

$$|\Psi\rangle = \int |p\rangle\langle p|\Psi\rangle dp = \int \tilde{\Psi}(p)|p\rangle dp \quad \rightsquigarrow |\tilde{\Psi}(p_0)|^2 dp = dP$$

Diskretno:

$$\rightarrow |\Psi\rangle = \sum_n |n\rangle\langle n|\Psi\rangle \ ; \quad P_n = |\langle n|\Psi\rangle|^2 = |C_n|^2$$

Od včeraj:

$$\langle x|p\rangle = f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x}$$ Lastno stanje $\hat{p}$

$$\langle x|x_0\rangle = \delta(x-x_0) = \Psi_{x_0}(x)$$ Lastno stanje $\hat{x}$

Krazi vektorji (nenormalizabilni npr.). V naravi ni takih stanj, lahko pa razvijemo po njih.

$$|x_0\rangle = \int \delta(x-x_0)|x\rangle dx \quad / \langle x_1|$$

$|x_0\rangle$ ↑ stanje v legi $x_0$; $\delta(x-x_0)$ ↑ verjetnostna amp. $\neq 0$ le v $x_0$; $|x\rangle$ ↑ vse lege

$$\langle x_1|x_0\rangle = \int \delta(x-x_0)\langle x_1|x\rangle dx =$$

$$= \int \delta(x-x_0)\delta(x-x_1) dx = \delta(x_1-x_0)$$

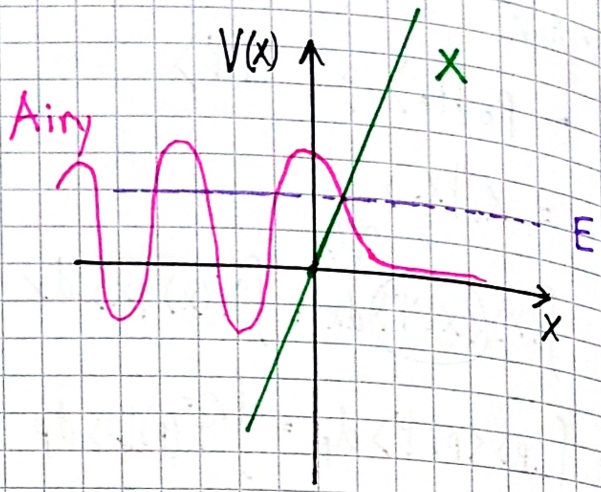
$$\Rightarrow \int \delta(x-x_0)\delta(x-x_1) dx = \delta(x_1-x_0)$$

$$\int (\delta(x-x_1))^2 dx = \ldots = \times$$ ne gre

# Primeri

- „prosti pad"

$$(-i\hbar\frac{\partial}{\partial x})^2 \rightarrow \frac{\hat{p}^2}{2m}\psi + mgx\psi = E\psi$$




$$\psi(x) = \int \tilde{\psi}(p)\,\frac{e^{i\frac{px}{\hbar}}}{\sqrt{2\pi\hbar}}\,dp$$

$$\frac{\hat{p}^2}{2m}|\psi\rangle + V(x)|\psi\rangle = E|\psi\rangle$$

$$\frac{p^2}{2m}\tilde{\psi} + mgi\hbar\frac{\partial\tilde{\psi}}{\partial p} = E\tilde{\psi}$$

$$\rightarrow \tilde{\psi}(p) = C\exp\left(\left(\frac{p^3}{6} + mE_p\right)\left(\hbar g m^2\right)\right)$$

- „Harmonski Oscilator"

## Harmonski Oscilator

$$H = E = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

Klasično: $\ddot{X} + \omega^2 X = 0$ ; $\omega^2 = \frac{k}{m}$

$X = X_0\cos(\omega t - \delta)$

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 = -\frac{\hbar^2 d^2}{2m\,dx^2} + \frac{1}{2}m\omega^2x^2 =$$

$$\xi^2 = \frac{\hbar}{\omega m}$$

$$= \frac{1}{2}\hbar\omega\left(\frac{x^2}{\xi^2} - \xi^2\frac{d^2}{dx^2}\right) =$$

Razlika kvadratov:

$a^2 - b^2 = (a-b)(a+b)$

$ab \neq ba$ sicer

$$= \frac{1}{4}\hbar\omega\left(\left(\frac{x}{\xi} + \xi\frac{d}{dx}\right)\left(\frac{x}{\xi} - \xi\frac{d}{dx}\right) + \left(\frac{x}{\xi} - \xi\frac{d}{dx}\right)\left(\frac{x}{\xi} + \xi\frac{d}{dx}\right)\right) = (*)$$

Vpeljimo:

$$\boxed{\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{x}{\xi} + \xi\frac{d}{dx}\right)}$$

Anihilacijski operator

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{i}{m\omega}p\right)$$

$$\boxed{a^\dagger = \frac{1}{\sqrt{2}}\left(\frac{x}{\xi} - \xi\frac{d}{dx}\right)}$$ Kreacijski operator

$$\left(\frac{d}{dx}\right)^\dagger = -\frac{d}{dx}$$

$$\Rightarrow x = \frac{\xi}{\sqrt{2}}(a + a^\dagger) = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$$

$$\frac{d}{dx} = \frac{1}{\xi\sqrt{2}}(a - a^\dagger) = i\sqrt{\frac{m\hbar\omega}{2}}(a^\dagger - a)$$

$$(*) = \Big(\underbrace{\left(\frac{x}{\xi} + \xi\frac{d}{dx}\right)}_{a}\underbrace{\left(\frac{x}{\xi} - \xi\frac{d}{dx}\right)}_{a^\dagger} + \left(\frac{x}{\xi} - \xi\frac{d}{dx}\right)\left(\frac{x}{\xi} + \xi\frac{d}{dx}\right)\Big)$$

$$\Rightarrow H = \frac{1}{2}\hbar\omega(aa^\dagger + a^\dagger a)$$

Vmesni račun:

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = \frac{1}{2}\left(\frac{x}{\xi} + \xi\frac{d}{dx}\right)\left(\frac{x}{\xi} - \xi\frac{d}{dx}\right) - \frac{1}{2}\left(\frac{x}{\xi} - \xi\frac{d}{dx}\right)\left(\frac{x}{\xi} + \xi\frac{d}{dx}\right)$$

$$= \frac{1}{2}\left(\frac{d}{dx}x - x\frac{d}{dx} + \frac{d}{dx}x - x\frac{d}{dx}\right) =$$ $\quad [x, -i\hbar\frac{d}{dx}] = i\hbar$

$$= \left[\frac{d}{dx}, x\right] = -\left[x, \left(-i\hbar\frac{d}{dx}\right)\frac{1}{-i\hbar}\right] = \frac{1}{i\hbar}i\hbar = 1$$

$$[a, a^\dagger] = 1$$

Nazaj:

$$\Rightarrow H = \frac{1}{2}\hbar\omega(\overbrace{aa^\dagger}^{a^\dagger a + 1} + a^\dagger a)$$

$$\Rightarrow \boxed{H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)}$$

Operator štetja

$$\hat{n} = a^\dagger a \; ; \; \hat{n}^\dagger = a^\dagger a = \hat{n}^\dagger$$

- $H = \hbar\omega\left(\hat{n} + \frac{1}{2}\right)$
- $\hat{n}|f_\lambda\rangle = \lambda|f_\lambda\rangle \quad / \cdot \langle f_\lambda|$

$$\langle f_\lambda|\hat{n}|f_\lambda\rangle = \langle f_\lambda|a^\dagger a|f_\lambda\rangle = \langle \underbrace{a f_\lambda|a f_\lambda}_{\geq 0}\rangle = \underset{\geq 0}{\lambda} \langle \underbrace{f_\lambda|f_\lambda}_{\geq 0}\rangle$$

$$\Rightarrow \quad \lambda \geq 0$$

Ali je $\lambda = 0$ rešitev?

$$a^\dagger a|f_0\rangle = 0$$

$$a|f_0\rangle = 0 \qquad \langle x|f_0\rangle = f_0(x)$$

$$\left(\frac{x}{q} + q\frac{d}{dx}\right) f_0(x) = 0$$

$$\Rightarrow \quad f_0(x) = \frac{1}{\sqrt{\sqrt{\pi}\, q}} e^{-\frac{1}{2}\frac{x^2}{q^2}}$$

funkcija za osnovno stanje

$\lambda = 0$ je rešitev

$[\hat{n}, a^\dagger]$

$$[\hat{n}, a^\dagger] = \underbrace{[a^\dagger a, a^\dagger]}_{1} + \underbrace{[a^\dagger, a^\dagger]}_{0} a = a^\dagger \qquad [\hat{n}, a^\dagger] = a^\dagger \ !$$

$$[\hat{n}, a] = [a^\dagger a, a] = a^\dagger [a, a] + [a^\dagger, a] a = -a \qquad [\hat{n}, a] = -a$$

Naj bo $\hat{n}|f_\lambda\rangle = \lambda|f_\lambda\rangle$ je rešitev.

$$\hat{n} a^\dagger|f_\lambda\rangle = (a^\dagger \hat{n} + a^\dagger)|f_\lambda\rangle = (\lambda+1) \underbrace{a^\dagger|f_\lambda\rangle}_{c_\lambda|f_{\lambda+1}\rangle}$$

$\Rightarrow$ Vsa cela nenegativna števila so rešitve

$$\lambda = 0, 1, 2, 3, \ldots = n$$

$$\langle a^\dagger f_\lambda|a^\dagger f_\lambda\rangle = |c_\lambda|^2 \langle f_{\lambda+1}|f_{\lambda+1}\rangle = \langle f_\lambda|a a^\dagger|f_\lambda\rangle \ ?$$

$$= \ldots ? \Rightarrow c_\lambda = \lambda + 1$$

Če je $|f_n\rangle$ normirana rešitev:

$$|f_{n+1}\rangle = \frac{1}{\sqrt{n+1}} a^+ |f_n\rangle$$

$$|f_n\rangle = \frac{a^+}{\sqrt{n+1-1}} |f_{n-1}\rangle$$

$$\vdots$$

$$\Rightarrow \boxed{|f_n\rangle = \frac{a^{+n}}{\sqrt{n!}} |f_0\rangle} \; ; \; |n\rangle = \frac{a^{+n}}{\sqrt{n!}} |0\rangle$$

Najnižje stanje pravimo tudi vakuum

$E_0 \neq 0$

$$\langle x | f_n \rangle = f_n(x) = \frac{1}{\sqrt{2^n n!}} \left( \frac{x}{\xi} - \xi \frac{d}{dx} \right)^n f_0(x)$$

$$a a^+ a^+ a^+ = (a^+ a + 1) a^+ a^+$$

$$a a^+ - a^+ a = 1$$

$$\langle f_m | x^4 | f_n \rangle = \langle x^2 f_m | x^2 f_n \rangle$$

$$x^2 |f_n\rangle = \frac{1}{2} (a + a^+)^2 \xi^2 \frac{a^{+n}}{\sqrt{n!}} |f_0\rangle$$

$$a^{+\,n+1} \; ; \; a (a^+)^n \; ; \; a |f_0\rangle = 0$$

Ali so $n = 0, 1, \dots$ vse rešitve?

$$[\hat{n}, a] = -a$$

$$\hat{n} a |n\rangle = (a \hat{n} - a) |n\rangle = (n-1) \underbrace{a |n\rangle}_{\propto |n-1\rangle}$$

$$\Rightarrow \boxed{\frac{a^n}{\sqrt{(n+1)!}} |f_n\rangle = |f_0\rangle}$$

Ali $\lambda = 7.2$? $\lambda = n + \nu$; $0 < \nu < 1$

$$\langle \hat{n} | f_\lambda \rangle = \lambda | f_\lambda \rangle = (n + \nu) | f_\lambda \rangle$$

$$\hat{n} a | f_\lambda \rangle = (n - 1 + \nu) a | f_\lambda \rangle$$

$\rightarrow$

$$\hat n a^2|f_\lambda\rangle = (n-2+\nu)\,a^2|f_\lambda\rangle$$
$$\vdots$$
$$\hat n a^n|f_\lambda\rangle = (n-n+\nu)\,a^n|f_\lambda\rangle$$
$$\hat n a^{n+1}|f_\lambda\rangle = (-1+\nu)\,a^{n+1}|f_\lambda\rangle$$

$$\nu - 1 < 0 \qquad \langle f_\lambda|\hat n|f_\lambda\rangle \geq 0$$

$$\Rightarrow \nu = 0 \qquad \hat n a^n|f_\lambda\rangle = 0 \qquad \Rightarrow n = 0,1,2,3,\dots$$
$$n\, a^{n+1}|f_\lambda\rangle = 0$$
$$\vdots$$

$$\Rightarrow \quad H = \hbar\omega\left(\hat n + \frac{1}{2}\right)$$
$$E_n = \hbar\omega\,(n + 1/2)$$

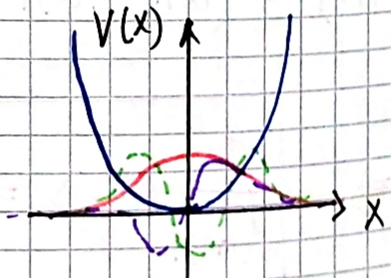
Posplošite: $\alpha = 1,2,3 \;;\; X_\alpha$ $\qquad m_\alpha\omega_\alpha^2$

$$H = \sum_{\alpha=1}^{N}\left(\frac{p_\alpha^2}{2m} + \frac{1}{2}k_\alpha X_\alpha^2\right)$$

$$H = \sum_\alpha \hbar\omega_\alpha\left(\hat n_\alpha + \frac{1}{2}\right) \;;\; [a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta}$$

Splošen harmonski oscilator

## Koherentno stanje




$$\Psi(x,t) = \psi_n(x) = e^{-i\frac{E_n}{\hbar}t}$$

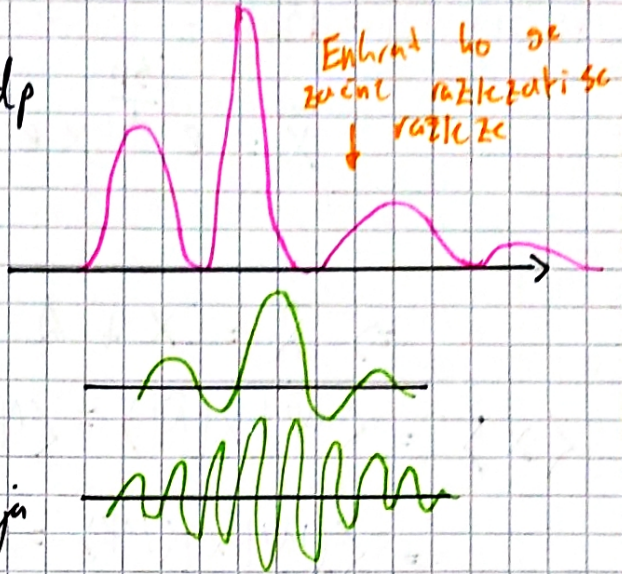
Zahtevamo:

$$a|f_\alpha\rangle = \alpha|f_\alpha\rangle \qquad \alpha = e^{i\delta}|\alpha| \in \mathbb{C}$$
$$\alpha \neq 0$$


Osnovno stanje za zamaknjen LHO izražen v bazi stanje

Valovni paket

$$\psi(x,t) = \int \tilde{\psi}(p)\, e^{\frac{ipx}{\hbar} - i\frac{p^2}{2m\hbar}t}\, dp$$

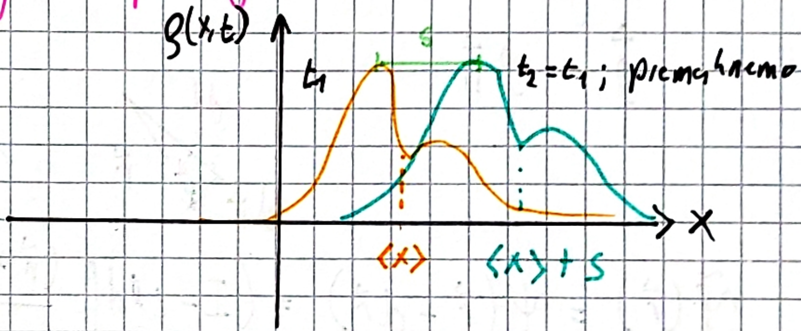



Hitrost paketa je skrita v valovni dolžini oz. frekvenci oscilacije znotraj ovojnice.

Interferenčne črte dobimo ker se del valovanja že odbija in interferira z prihajajočim.

# Simetrije
## (in simetrijske operacije)

- Translacija (premik)




$$U(s)\psi(x) = \tilde{\psi}(x) = \psi(x-s) =$$

Translirano, ne FT !

$$= \psi(x) - s\frac{d}{dx}\psi + \frac{s^2}{2!}\frac{d^2\psi}{dx^2} = \left(1 - s\frac{d}{dx} + \dots\right)\psi(x) =$$

$$= \underbrace{e^{-s\frac{d}{dx}}}_{U}\psi(x) \qquad U(s) = e^{-\frac{isp}{\hbar}}$$

(Unitarni) operator premika

V splošnem:

$$U(\vec{a}) = e^{-i\frac{\vec{a}\cdot\vec{p}}{\hbar}} = e^{iK} \; ; \; K = K^{T}$$

$\vec{p}$ ... generator transformacije

Vmesna vaja: Baker-Hausdorffova lema

$$\tilde{X} = e^{\frac{isp}{\hbar}} X e^{-\frac{isp}{\hbar}} = X + [\underbrace{i\frac{sp}{\hbar}}_{S}, X] + \frac{1}{2}\left[\frac{isp}{\hbar}, \left[\frac{isp}{\hbar}, X\right]\right] + \dots$$

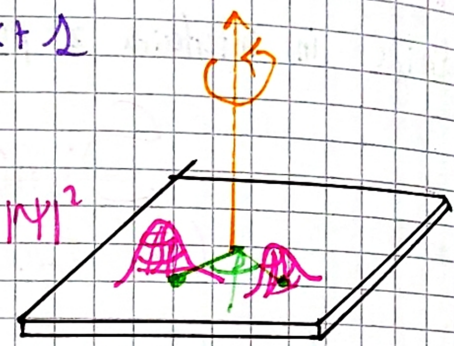
$$\Rightarrow \tilde{X} = X + \Delta$$

$$\langle X \rangle = \langle \tilde{\Psi} | X | \tilde{\Psi} \rangle = \langle \Psi(x-s) | x | \Psi(x-s) \rangle =$$

$$= \langle U\Psi | x | U\Psi \rangle = \langle \Psi | U^{+} x U | \Psi \rangle =$$

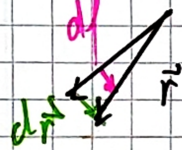
$\tilde{X} = X + \Delta$

$$= \langle x \rangle \Big|_{\Delta = 0} + \Delta.$$




·· Rotacija (vrtenje)

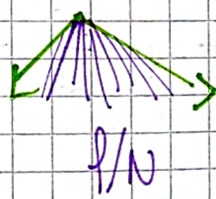
$$\vec{\varphi} = \varphi \vec{n}$$




$d\vec{r} = d\varphi\, \vec{n} \times \vec{r}$

$$\tilde{\Psi}(\vec{r}) = \Psi(\vec{r} - d\vec{r}) = \left(I - i\, d\varphi \frac{(\vec{n} \times \vec{r}) \cdot \vec{p}}{\hbar} + \mathcal{O}(d\varphi^2)\right) \Psi(\vec{r})$$

$$U(\varphi) = \lim_{N \to \infty} \left(I - i \frac{\varphi}{N} \frac{(\vec{n} \times \vec{r}) \cdot \vec{p}}{\hbar}\right)$$




$$(\vec{n} \times \vec{r}) \cdot \vec{p} = \vec{n} \cdot (\vec{r} \times \vec{p}) = \vec{n} \cdot \vec{L}$$

$$\vec{L} = \vec{r} \times \vec{p} = L^{\dagger}$$

$$\lim_{N \to \infty} \left(1 + \frac{X}{N}\right)^{N} = e^{X}$$

$$\Rightarrow \underline{\underline{U(\varphi) = e^{-i\varphi \frac{\vec{n} \cdot \vec{L}}{\hbar}}}}$$

## Inverzija prostora (parnost)

$$\mathcal{P} f(\vec{r}) \to f(-\vec{r}); \quad \vec{r} \to -\vec{r}$$

$$\mathcal{P}: \quad \vec{r} \to -\vec{r}$$
$$\nabla \to -\nabla$$
$$\nabla^2 \to \nabla^2$$
$$V(\vec{r}) \overset{?}{\to} V(-\vec{r})$$

Naj velja $V(\vec{r}) = V(-\vec{r})$; $V(x) = V(-x)$. V stacionarnem stanju:

$$H\psi(x) = E\psi(x)$$

$$\mathcal{P} H\psi = H\mathcal{P}\psi = E\mathcal{P}\psi$$

$$\mathcal{P}V = V\mathcal{P}$$
$$\mathcal{P}H = H\mathcal{P}$$

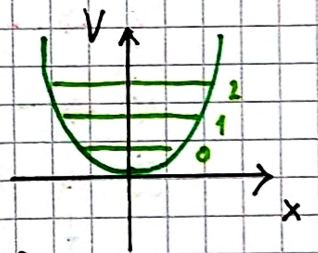
Očitno, če je $\psi$ rešitev je tudi $\mathcal{P}\psi$.

$$\psi_\pm = \frac{1}{\sqrt{2}}\left(\psi(\vec{r}) \pm \psi(-\vec{r})\right);$$

$$\mathcal{P}\psi_\pm = \pm\psi_\pm$$

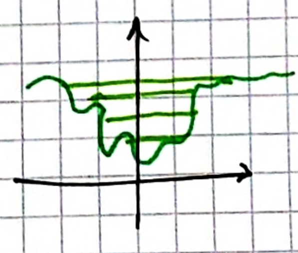
Če $E$ ni degeneriran: $\psi$ je soda ali liha.

$$\left(\mathcal{P}\psi_n = (-1)^n \psi_n\right)$$
$$\psi_0 \sim e^{-x^2}$$
$$\psi_n \sim a^\dagger \psi_0 \sim \left(x + \frac{\partial}{\partial x}\right)\psi_0$$

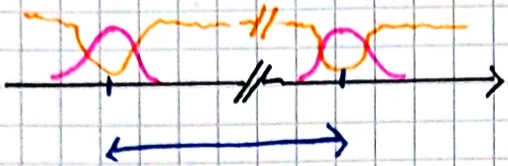



Degeneriranc zato samo ena rešitev za vsak $n$.

Vezana stanja (energija v neskončnosti je manjša od potenciala) imajo energijo, ki ni degenerirana.



V tem primeru imamo formalno dve ~~d~~ nedegenerirani VF ampak ker katko

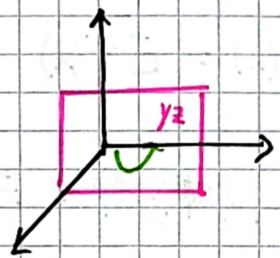



naredimo lin. komb. je to degenerirano. To je patološki primer.

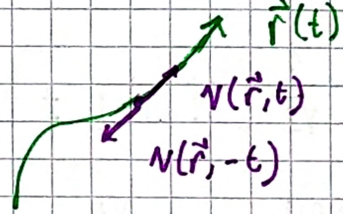
V 1D je energija nedegenerirana in za sod potencial so VF sode ali lihe.

## :: Zrcaljenje

$$\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} -x \\ y \\ z \end{pmatrix}$$




## :: Obrat časa




$\vec{v} = \frac{d}{dt}\vec{r}$

Klasično: $m\frac{d^2\vec{r}(t)}{dt^2} = \vec{F}(\vec{r},t)$

$t \to -t$

$\vec{v} \to -\vec{v}$

$\vec{a} \to \vec{a}$ ; če $\vec{F} \neq \vec{F}(t)$ je $\vec{r}(-t) = \vec{r}(t)$

$$\frac{d^2\vec{r}(t)}{d(-t)^2} = \frac{d^2\vec{r}(t)}{dt^2}$$

Čisto v resnici v klasičnem zaradi entropijskega zakona niso obrati simetrične na čas. Recimo zračni upor pri poševnem metu (sistem več teles). Bistvo entropijskega zakona je, da ne moremo obrniti časa.

Kvantno: Predpostavimo $V(\vec{r})$ in ne $V(\vec{r},t)$. Iz Schrödingerjeve enačbe

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = H\Psi(\vec{r},t)$$

$$t \rightarrow -t$$

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial(-t)} = H\Psi(\vec{r},-t) \Big/^{*}$$

Predpostavimo $H^{*} = H$

$$+i\hbar \frac{\partial \Psi^{*}(\vec{r},-t)}{\partial(+t)} = H\Psi^{*}(\vec{r},-t)$$

!

Sakurai ugiga o kvantni mehaniki

Če je $\Psi(\vec{r},t)$ rešitev je $\Psi^{*}(\vec{r},t)$ tudi rešitev.

Sakurai: Operator obrata časa → op. spremembe smeri gibanja predlaga

↳ (Da ni kot v znanstveni fantastiki)

$$\mathcal{T}\Psi = \Psi^{*}\ ;\ \underline{\underline{\mathcal{T} = K\ ;\ Kz = z^{*}K}}\ ;\ z \in \mathbb{C}$$

$$\Psi(\vec{r},t) \rightarrow \mathcal{T}\Psi(\vec{r},-t)$$

↳ To vstavimo ročno!

↑ Poskrbi samo za $*$

V klasični mehaniki ta operator nič ne naredi $\mathcal{T} = I$

Primer:

1). $$\Psi_p = e^{+i\frac{p}{\hbar}x - i\frac{E}{\hbar}t} = \Psi_p(x,t)$$ Ravni val

$$\Psi(x,t) \longrightarrow \tilde{\Psi}(x,t) = \mathcal{T}\Psi(x,-t) = \Psi_{-p}(x,-t) =$$

$$= e^{-i\frac{p}{\hbar}x - (-1)(-i)\frac{E}{\hbar}t} =$$

$$= e^{-i\frac{p}{\hbar}x - i\frac{E}{\hbar}t}$$

2.) Stacionarno stanje $\psi(\vec{r})$

$$H\psi = E\psi \quad / \ \mathcal{T}$$

$$H\mathcal{T}\psi = \mathcal{T}H\psi = E\mathcal{T}\psi$$ $\Rightarrow$ Če je $\psi$ rešitev je tudi $\psi^*$ rešitev. Spet

Tako lahko sestavimo rešitev:

$$\tilde{\psi} = \frac{1}{\sqrt{2}}(\psi + \psi^*)$$

Če energija ni degenerirana je

$$\psi = e^{i\delta}\tilde{\psi} \, ; \ \tilde{\psi} \in \mathbb{R}$$ !

(in je $H$ invarianten na obrat časa) so rešitve realne.

To ne velja, če imamo magnetna polja

$$\vec{F} = e\vec{v}\times\vec{B} + e\vec{E}$$
$$\vec{B} \to -\vec{B}$$

# Vrtilna količina

• $\frac{d}{dt}\langle\underbrace{(\vec{r}\times\vec{p})}_{\vec{L}}\rangle = \langle\vec{M}\rangle$ ; $\quad \vec{r}\times\vec{F} = \vec{r}\times(-\nabla V)$

$$\vec{\varphi} = \varphi\vec{n}$$

•• $U = e^{-i\varphi\vec{n}\cdot\vec{L}} = U(\vec{\varphi})$

$(AB)^\dagger = B^\dagger A^\dagger$

$x_\alpha p_\beta = p_\beta x_\alpha$

Vpeljimo operator vrtilne količine: $\boxed{\vec{L} = \vec{r}\times\vec{p}}$

Vprašamo se ali je Hermitski? Ja. $\vec{L} = \vec{L}^\dagger$

$$[x_\alpha, p_\beta] = i\hbar\delta_{\alpha\beta}$$ $\quad \vec{L} = (L_x, L_y, L_z)$

Zgleda trivial ampak ni:

$$\vec{L} = \vec{r}\times\underset{\substack{\uparrow\\ \text{gradient}}}{\vec{p}} = -\underset{\substack{\uparrow\\ \text{vloga rotorja}}}{\vec{p}}\times\vec{r} = \vec{L}^\dagger$$