Pričakovane vrednosti

$$X_t = \int_{-\infty}^{\infty} x \rho(x,t)\, dx$$

težišče porazdelitve verjetnosti

↳ $X_t = X_t(t)$ • se giblje

$$\langle x \rangle = \int \psi^* x \psi \, dx$$

pričakovana vrednost
"
srednja vrednost

↳ zanimivo je kako se $\langle x \rangle$ s časom spreminja:

$$\frac{d\langle x\rangle}{dt} = \langle v \rangle = \int \left[\frac{\partial \psi^*}{\partial t} x\psi + \psi^* x \frac{\partial \psi}{\partial t}\right] dx$$

hitrost težišča porazdelitve

rabimo:

iz Schrö. enačbe: $\frac{\partial \psi}{\partial t} = -\frac{\hbar}{i2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{V}{i\hbar}\psi$

$$\frac{\partial \psi^*}{\partial t} = \frac{\hbar}{2im}\frac{\partial^2 \psi^*}{\partial x^2} + \frac{V^*}{-i\hbar}\psi^*$$ → zgornjo enačbo konjugiramo

torej: $\langle v \rangle = \frac{\hbar}{2im}\int \left[\frac{\partial^2 \psi^*}{\partial x^2} x\psi - \psi^* x \frac{\partial^2 \psi}{\partial x^2}\right] dx$

↳ vmes dobiš $\psi^* V \psi - \psi V^* \psi^* =$ ... V = realen

poskušamo sprovocit na odvod nečesa: $\frac{\partial^2 \psi^*}{\partial x^2} x\psi = \frac{\partial}{\partial x}\left(\frac{\partial \psi^*}{\partial x} x\psi\right) - \frac{\partial \psi^*}{\partial x}\psi - \frac{\partial \psi^*}{\partial x} x \frac{\partial \psi}{\partial x} =$

$\frac{\partial x}{\partial x} = 1$

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

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

↳ je enako kot 2. člen v izrazu za $\langle v \rangle$!

Torej: $\langle v \rangle = \frac{\hbar}{2im}\int_{-\infty}^{\infty} \frac{\partial}{\partial x}\Big(\underbrace{\frac{\partial \psi^*}{\partial x} x\psi - \psi^* x \frac{\partial \psi}{\partial x}}_{x \cdot j} - \overbrace{\psi^* \psi}^{\rho}\Big) dx + \frac{\hbar}{2im} \cdot 2\int_{-\infty}^{\infty} \psi^* \frac{\partial}{\partial x}\psi \, dx$

$j(\infty) = 0$, $j(-\infty) = 0$; $\rho(\infty) = 0$, $\rho(-\infty) = 0$!

$$\underset{\substack{\| \\ m\frac{d\langle x\rangle}{dt}}}{\overset{\substack{\langle p \rangle \\ \|}}{m\langle v \rangle}} = \int \psi^* \left(-i\hbar\frac{\partial}{\partial x}\right)\psi \, dx$$

$\psi = \psi(x,t)$

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

$$\langle p\rangle = \int \psi^* \hat{p} \psi \, dx = \int (\hat{p}\psi)^* \psi \, dx$$

$\langle x\rangle = \langle x\rangle^*$ je realno.

Poglejmo: $\langle p\rangle - \langle p\rangle^* = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right)\psi \, dx - \int \psi \left(i\hbar \frac{\partial}{\partial x}\right)\psi^* dx$

$$= \frac{\hbar}{i} \int \underbrace{\left(\psi^* \frac{\partial \psi}{\partial x} + \psi \frac{\partial \psi^*}{\partial x}\right)}_{\frac{\partial}{\partial x}|\psi|^2_{\rho}} dx =$$

$$\langle p\rangle - \langle p\rangle^* = \frac{\hbar}{i} \rho(x,t) \Big|_{-\infty}^{\infty} = 0$$

$\langle p\rangle = \langle p\rangle^*$

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

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

če imam: $f(x) = \sum_n c_n x^n \Rightarrow$ definiram $f(\hat{p}) := \sum_n c_n \hat{p}^n$

vidimo: $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = \frac{\hat{p}^2}{2m}$

No pa sestavimo operator $\hat{H} = \underbrace{\frac{\hat{p}^2}{2m}}_{\hat{T}} + \hat{V}$

$\langle H\rangle = \int \psi^* \hat{H} \psi \, dx = \langle H\rangle^*$ → tole bo treba pokazat.

$\int \psi (\hat{H}\psi)^* dx$

vzemimo nek φ in ψ → valovni funkciji

Pokažimo tole: $\int_{-\infty}^{\infty} \varphi^* H \psi \, dx = \int (H\varphi)^* \psi \, dx$ za $\forall \varphi, \psi \in L_2$

poglejmo: $\int \varphi^* \frac{\partial^2}{\partial x^2} \psi \, dx = \underbrace{\varphi^* \frac{\partial \psi}{\partial x} \Big|_{-\infty}^{\infty}}_{0} - \int \frac{\partial \varphi^*}{\partial x} \frac{\partial \psi}{\partial x} dx =$

$\int u\,dv = uv - \int v\,du$

še enkrat per partes

$$= \psi^* \frac{\partial \psi}{\partial x}\Big|_{-\infty}^{\infty} - \psi \frac{\partial \psi^*}{\partial x}\Big|_{-\infty}^{\infty} + \int \frac{\partial^2 \psi^*}{\partial x^2} \psi \, dx$$

torej :

$$\int \psi^* \frac{\partial^2}{\partial x^2} \psi \, dx = \int \frac{\partial^2 \psi^*}{\partial x^2} \psi \, dx$$

$\hookrightarrow$ je hermitski operator $\square$ to je to.

Kaj pa pospešek? Pokazali bomo, da tudi v kvantni velja $F = ma$.

$$A \psi(x,t) = \psi_1(x,t)$$

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

$$\frac{d}{dt}\langle A \rangle = \frac{d}{dt} \int \psi^* A \psi \, dx = \int \frac{\partial \psi^*}{\partial t} A \psi \, dx +$$

$$+ \int \psi^* \frac{\partial A}{\partial t} \psi \, dx + \int \psi^* A \frac{\partial \psi}{\partial t} dx =$$

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

prejsmo pokazali, da gre H lahko k ψ

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} H \psi \qquad H = \frac{\hat{p}^2}{2m} + V$$

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

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

$$= \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{i}{\hbar} \langle [H, A] \rangle$$

$[H, A] := HA - AH \rightarrow$ komutator. Ima vse lastnosti, ki jih ima Poissonov oklepaj.

DN! Preveri :

1) $[AB, C] = A[B, C] + [A, C]B$

2) Jakobi : $[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$

3) Baker - Haussdorffov Lema :

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

$$\frac{d\langle H\rangle}{dt} = \left\langle \frac{\partial H}{\partial t} \right\rangle \quad ; \text{ker } [H,H]=0$$

! če je V konst, $V \neq V(t)$, je $\langle H\rangle$ konst.

DISPERZIJA, VARIANCA, NEDOLOČENOST, 2. moment

znamo izračunat : $\langle A\rangle$

$$\langle (A-\langle A\rangle)^2\rangle = \langle A^2 - 2A\langle A\rangle + \langle A\rangle^2\rangle$$
$$= \langle A^2\rangle - \langle A\rangle^2 := (\Delta A)^2$$

imejmo še: $\langle B\rangle \quad (\Delta B)^2 = \langle B^2\rangle - \langle B\rangle^2$

iz tega se da pokazati, da:

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

→ Schwarz: $f,g \in L_2$

$$\left(\int f^* g \, dx\right)^2 \geq \int |f|^2 dx \int |g|^2 dx$$

to uporabiš za dokazat

Gremo zdaj k fiziki:

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

$\langle x\rangle$

$\langle v\rangle$

Poglejmo $\frac{d}{dt}\langle v\rangle = \frac{d}{dt}\frac{\langle p\rangle}{m} = \frac{1}{m}\frac{d}{dt}\langle p\rangle = \frac{1}{m}\frac{i}{\hbar}\langle [H,p]\rangle$

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

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

$$[p^2, p] = 0$$

$$[V,p]\psi = \underbrace{V\left(-i\hbar\frac{\partial}{\partial x}\psi\right)}_{Vp\psi} - \underbrace{\left(-i\hbar\frac{\partial}{\partial x}\right)V\psi}_{pV\psi} = i\hbar\left(\frac{\partial V}{\partial x}\right)\psi$$

$$\left(-i\hbar\right)\left[\frac{\partial V}{\partial x}\psi + V\frac{\partial \psi}{\partial x}\right]$$

$$\langle a\rangle = \frac{d}{dt}\langle v\rangle = \frac{1}{m}\frac{i}{\hbar}\left\langle (i\hbar)\left(\frac{\partial V}{\partial x}\right)\right\rangle =$$

Ehrenfestov teorem

$$= \frac{1}{m}\underbrace{\frac{i}{\hbar}(i\hbar)}_{-1}\underbrace{\int \psi^* \frac{\partial V}{\partial x}\psi \, dx}_{\langle \frac{\partial V}{\partial x}\rangle} \Rightarrow m\langle \vec{a}\rangle = -\langle \nabla V\rangle = \langle \vec{F}(\vec{r},t)\rangle$$

$$\langle \vec{F}\rangle \neq \vec{F}(\langle \vec{r}\rangle, t)$$

$$m\langle\vec{a}\rangle = -\langle\nabla V\rangle = \langle\vec{F}(\vec{r},t)\rangle \neq \vec{F}(\langle\vec{r}\rangle,t)$$

→ to ni invariantno na Lorentzove transf. Ni relativistična enačba.

Zdej, če je $(\Delta\vec{r})^2 \to 0$, je $\langle\vec{F}(\vec{r},t)\rangle = \vec{F}(\langle\vec{r}\rangle,t)$

↳ to je v klasični

tu mi v tej enačbi nobenega $\hbar$...

ENERGIJA

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

Poglejmo stacionarno stanje:

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

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

ker $e^{-i\frac{E}{\hbar}t}$ nima opravka z H

$$\langle H\rangle = \int\Psi^*(x,t)\,H\,\Psi(x,t)\,dx = \int\psi^*(x)\underbrace{\hat{H}\psi(x)}_{=E\psi}\,dx = E$$ juhu.

Stacionarna stanja imajo energijo $E = \langle H\rangle$.

Koliko je $\langle H^2\rangle = ?$

$$\langle H^2\rangle = \int\psi^*(x)\,H\,E\psi(x)\,dx = E^2$$

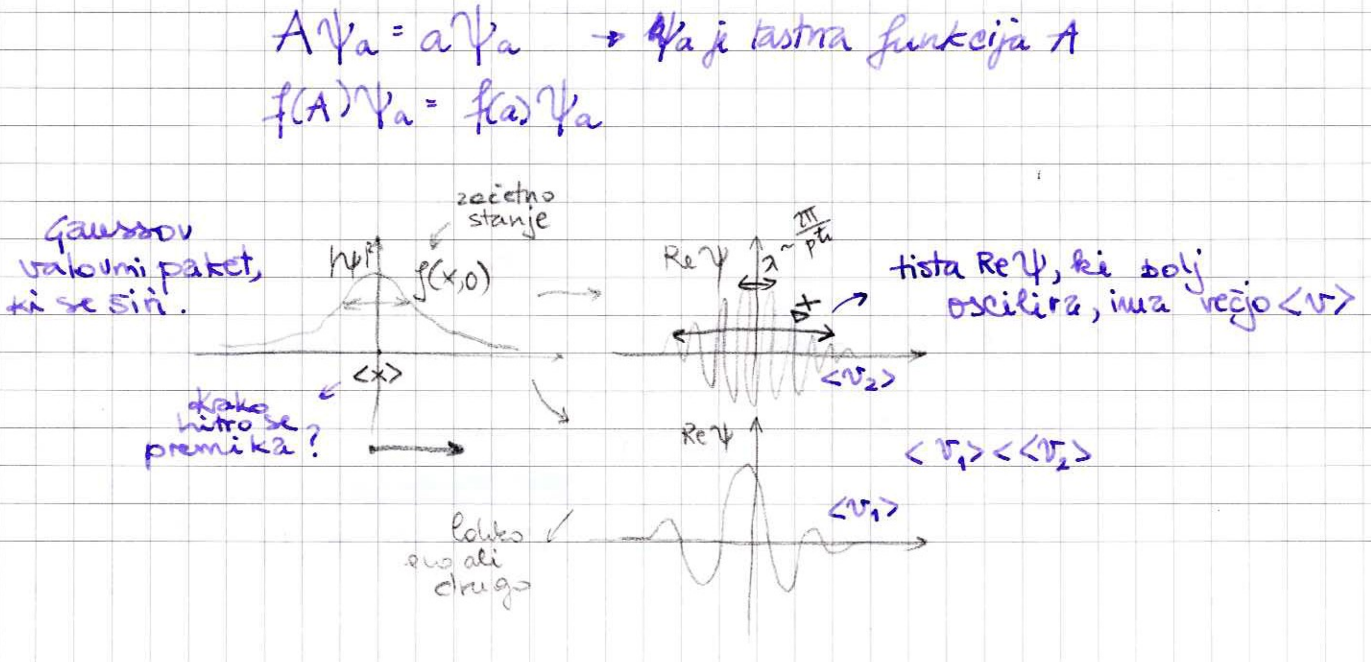
$$\langle H^n\rangle = E^n$$

$\langle f(H)\rangle = f(E)$ → to velja za stacionarne funkcije

$$(\Delta E)^2 = \langle H^2\rangle - \langle H\rangle^2 = 0$$

$A\psi_a = a\psi_a$ → ψ_a je lastna funkcija A

$$f(A)\psi_a = f(a)\psi_a$$



↗ če imamo podan $\psi(x,0)$, lahko računamo kako hitro se premika.

za $V=0 \Rightarrow \frac{d\langle p\rangle}{dt} = \frac{i}{\hbar}\langle[\frac{p^2}{2m}, p]\rangle = 0$ → hitrost je konst.

Heisenberg:

$$\Delta x \Delta p \geq \frac{1}{2}|\langle[x,p]\rangle|$$

$$[x,p]\psi = x(-i\hbar\frac{\partial}{\partial x}\psi) - (-i\hbar\frac{\partial}{\partial x})x\psi =$$

$$= i\hbar\psi$$

➡ $[x,p] = i\hbar$ v Poissonovih oklepajih: $[q_i, p_j] = \delta_{ij}$

↳ posplošimo:

$[r_e, p_j] = i\hbar\delta_{ej}$

Torej: $\Delta x \Delta p \geq \frac{\hbar}{2}$ → za Gaussov paket je $\Delta x \Delta p = \frac{\hbar}{2}$. za ostale je več.

Informacije o delcu:

$\langle x\rangle$, Δx → kje je kako je razmazan

λ, $\langle p\rangle$, Δp → kako hitro se giblje in kako je to nejasno

Časovni razvoj $\psi(x,t)$

$\psi(x,0)$ poznamo.

Vprašanje je kakšen je $\psi(x,t) = ?$

Recimo, da znamo: $\psi(x,0) = \sum_n C_n \varphi_n(x)$; $H\varphi_n = E_n\varphi_n$ → φ_n so lastne funkcije

$\Phi_n(x,t) = e^{-i\frac{E_n}{\hbar}t}\varphi_n(x)$ recimo, da velja: $\int \varphi_m^* \varphi_n \, dx = \delta_{mn}$

In v kvantni 3 postulat, da se da to vedno storit.

$$\rightarrow \int \varphi_m^*(x)\,\psi(x,0)\,dx = c_m$$

torej: $$\Psi(x,0) = \sum_m \int_{-\infty}^{\infty} \varphi_n^*(x')\,\psi(x',0)\,dx'\,\varphi_n(x) =$$

$$= \int_{-\infty}^{\infty} \underbrace{\Big(\sum_m \varphi_n^*(x')\,\overset{\Phi_n(x,0)}{\varphi_n(x)}\Big)}_{\delta(x-x')} \psi(x',0)\,dx'$$

vprašanje je kako izgleda $\psi(x,t) = ?$

ker vemo: $H\varphi_n = E_n\varphi$

$f(H)\varphi_n = f(E_n)\,\varphi_n$

$$\psi(x,t) = \sum_m c_m\,\Phi(x,t) = \sum c_n e^{-i\frac{E_n}{\hbar}t}\varphi_n(x)$$

$$e^{-i\frac{E_n}{\hbar}t} = e^{-i\frac{\hat{H}}{\hbar}t}$$

$$\rightarrow e^{-\frac{\partial^2}{\partial x^2}} = 1 - \frac{\partial^2}{\partial x^2} + \ldots + \frac{1}{n!}\ldots$$

$$= \sum c_n e^{-i\frac{\hat{H}}{\hbar}t}\varphi_n(x)$$

$$= e^{-i\frac{\hat{H}}{\hbar}t} \underbrace{\sum_n c_n\varphi_n(x)}_{\Psi(x,0)} = e^{-i\frac{\hat{H}}{\hbar}t}\Psi(x,0)$$

$$\Psi(x,t) = \underbrace{e^{-i\frac{\hat{H}}{\hbar}t}}_{\text{Operator časovnega razvoja}}\Psi(x,0)$$

Operator časovnega razvoja = zapisan z vrsto

DN!
Pojdi čez vse korake.