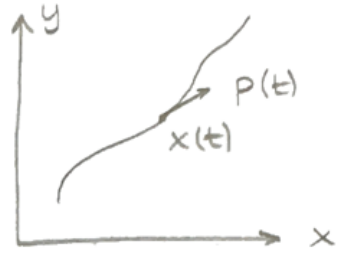
6/9-18 Föreläsning 2

Vågfunktion och Schrödingerekvationen

Tillstånd: Klassisk mekanik $\rightarrow \{x, v\}$
positionen, x och $\{x, p\}$
rörelsemängden, p hos en partikel
bestämmer tillståndet.

Vi vill hitta positionen x som en funktion av tiden: $x(t)$. Vi bestämmer $x(t)$ från Newtons II:a lag:

$$m\frac{d^2x}{dt^2} = F \quad , \quad F = ma$$



$$\Rightarrow \quad P = \frac{dx}{dt} \cdot m \quad \Rightarrow \quad \{x(t), p(t)\}$$

Kvantmekanik: $\Psi(x,t)$

Tidsutvecklingen av $\Psi(x,t)$:

$$\boxed{i\hbar\frac{\partial\Psi}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - V\Psi = 0}$$ där V är yttre potential

Schrödingerekvationen (SE)

Linjär vågekvation: Om Ψ_A och Ψ_B är lösningar till SE $\Rightarrow a\Psi_A + b\Psi_B$ lösning till SE, (a, b - konst.)

Att lösa SE:

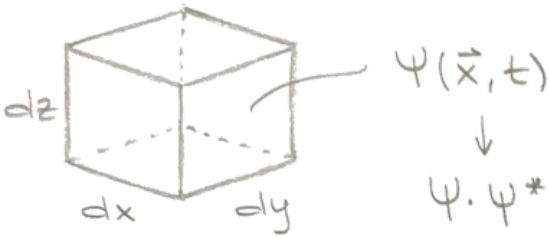
Givet $\Psi(x,0) \Rightarrow$ SE ger oss lösningen $\Psi(x,t)$.

$\{x(t), p(t)\} \longleftrightarrow \Psi(x,t)$?

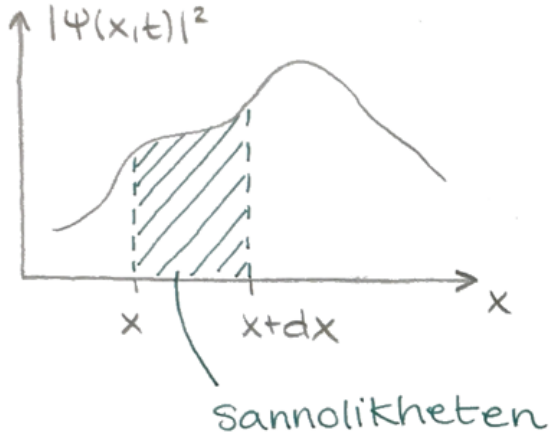
Hur kan $\Psi(x,t)$ beskriva en partikel?

Borns statistiska tolkning

$|\Psi(x,t)|^2 dx$ = sannolikheten att hitta partikeln i intervallet $[x, x+dx]$



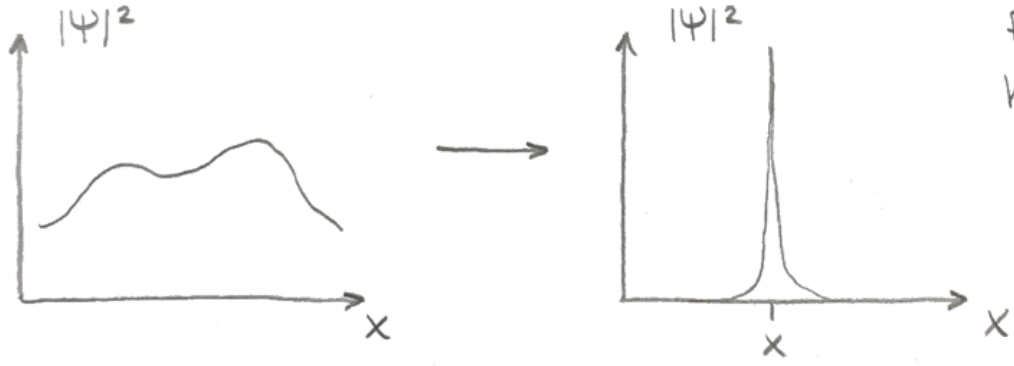
1D:



Normera $\Psi(x,t)$ s.a

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$

När vi mäter en partikels position: (att mäta positionen påverkar sannolikhetskurvan)



MEN sannolikheten måste bevaras!

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 0 \quad ?$$

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} |\Psi(x,t)|^2 dx$$

$$\frac{\partial}{\partial t}|\Psi(x,t)|^2 = \frac{\partial}{\partial t}(\Psi \cdot \Psi^*) = \frac{\partial \Psi}{\partial t}\Psi^* + \Psi\frac{\partial \Psi^*}{\partial t}$$

$$\text{SE:} \quad \left.\begin{aligned} \frac{\partial \Psi}{\partial t} &= \frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi \\ \frac{\partial \Psi^*}{\partial t} &= -\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^* \end{aligned}\right\}$$

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

$$+ \Psi\left(-\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{h}V\Psi^* = \frac{i\hbar}{2m}\left(\frac{\partial^2 \Psi}{\partial x^2}\Psi^* - \Psi\frac{\partial^2 \Psi^*}{\partial x^2}\right) =$$

$$= \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\right]$$

$$\Rightarrow \frac{d}{dt}\int_{-\infty}^{\infty}|\Psi|^2 dx = \int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\right]dx$$

$$= \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\Bigg|_{-\infty}^{\infty} = 0$$

Väntevärdet

Givet en funktion f så ges dess väntevärde av

$\langle f \rangle = \int_{-\infty}^{\infty} f|\Psi|^2 dx$, $\langle f \rangle$ är ett ensambelmedelvärde.

Väntevärdet av en funktion, f, är medelvärdet av ett stort antal mätningar på identiska system.

Väntevärdet av positionen:

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\Psi|^2 dx$$

$$\Rightarrow \frac{d\langle x\rangle}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} x|\psi|^2\,dx = \int_{-\infty}^{\infty} x\,\frac{\partial|\psi|^2}{\partial t}\,dx =$$

$$= \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)dx =$$

Schrödingerekvationen

partialintegration

$$= -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left(\psi^*\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\psi\right)dx =$$

$$= -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}\,dx$$

Väntevärdet av rörelsemängden:

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}\,dx$$

Skriv detta som:

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

x och p är operatorer: $x \rightarrow x$

$p \rightarrow -i\hbar\frac{\partial}{\partial x}$

Alla klassiska dynamiska variabler, t.ex. kinetisk energi, kan skrivas som funktioner av (x, p).

$\Rightarrow$ metod att beräkna väntevärdet för alla klassiska dynamiska storheter.

Klassisk dynamisk variabel: $F = F(x, p)$

$$\langle F \rangle = \int_{-\infty}^{\infty} \psi^* F\left(x, -i\hbar \frac{\partial}{\partial x}\right) \psi \, dx$$

Ex. kinetisk energi $T = \frac{mv^2}{2} = \frac{p^2}{2m}$

$\Rightarrow$ väntevärdet $\langle T \rangle = \int_{-\infty}^{\infty} \psi^* \frac{1}{2m} \left(-i\hbar \frac{\partial}{\partial x}\right)^2 \psi \, dx =$

$$= \int_{-\infty}^{\infty} \psi^* \frac{1}{2m} \left(-i\hbar \frac{\partial}{\partial x}\right)\left(-i\hbar \frac{\partial \psi}{\partial x}\right) dx$$

$$\langle T \rangle = \frac{1}{2m} \int_{-\infty}^{\infty} \psi^* (-i\hbar)^2 \frac{\partial}{\partial x}\left(\frac{\partial \psi}{\partial x}\right) dx = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \psi^* \frac{\partial^2 \psi}{\partial x^2} \, dx$$

Newtons II:a lag

$$\frac{dp}{dt} = F = -\frac{\partial V}{\partial x}$$

konservativa krafter

$$\langle p \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial x} \, dx$$

$$\frac{d\langle p \rangle}{dt} = -i\hbar \frac{d}{dt} \int \psi^* \frac{\partial \psi}{\partial x} \, dx = -i\hbar \int \frac{\partial}{\partial t}\left[\psi^* \frac{\partial \psi}{\partial x}\right] dx$$

$$= -i\hbar \int \left[\frac{\partial \psi^*}{\partial t} \frac{\partial \psi}{\partial x} + \psi^* \frac{\partial}{\partial x}\left(\frac{\partial \psi}{\partial t}\right)\right] dx$$

$$= -i\hbar \int \left[-\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar} V \psi^*\right] \frac{\partial \psi}{\partial x} \, dx - i\hbar \int \psi^* \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \right.$$

$$\left. - \frac{1}{\hbar} V \psi\right] dx$$

$$\frac{d\langle p\rangle}{dt} = -\frac{\hbar^2}{2m}\int \underbrace{\left(\frac{\partial^2\psi^*}{\partial x^2}\cdot\frac{\partial\psi}{\partial x} - \psi^*\frac{\partial^3\psi}{\partial x^3}\right)}_{= \frac{\partial}{\partial x}\left[\left|\frac{\partial\psi}{\partial x}\right|^2 - \psi^*\frac{\partial^2\psi}{\partial x^2}\right] \xrightarrow[x\to\infty]{} 0} dx -$$

$$-\int_{-\infty}^{\infty}\frac{\partial V}{\partial x}|\psi|^2 dx$$

$$\Rightarrow \frac{d\langle p\rangle}{dt} = -\int_{-\infty}^{\infty}\frac{\partial V}{\partial x}|\psi|^2 dx = -\left\langle\frac{\partial V}{\partial x}\right\rangle$$