Vi beviser uskarphetsrelasjonen:

$$(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \langle (\hat{A} - \langle A \rangle)^2 \rangle \equiv \langle \tilde{A}^2 \rangle \qquad (\text{da } \langle \hat{A} \rangle = \langle A \rangle)$$

$$(\Delta B)^2 = \langle (\hat{B} - \langle B \rangle)^2 \rangle \equiv \langle \tilde{B}^2 \rangle$$

"Triks": Se på $\int |\tilde{A}\Psi + i\alpha \tilde{B}\Psi|^2 dx$, som åpenbart er ≥ 0, og med vilkårlig, reell α i første omgang.

Har reelle A og B, dvs hermiteske $\hat{A}, \hat{B}$ og $\tilde{A}, \tilde{B}$, så vi kan bruke PCH 2.8 etter behov.

$$\int (\tilde{A}\Psi + i\alpha\tilde{B}\Psi)^* (\tilde{A}\Psi + i\alpha\tilde{B}\Psi)\, dx \geq 0$$

$$\Rightarrow \int (\tilde{A}\Psi)^* \tilde{A}\Psi\, dx + \alpha^2 \int (\tilde{B}\Psi)^* \tilde{B}\Psi\, dx$$
$$+ i\alpha \int (\tilde{A}\Psi)^* \tilde{B}\Psi\, dx - i\alpha \int (\tilde{B}\Psi)^* \tilde{A}\Psi\, dx \geq 0$$

Bruker PCH 2.8 til å få alt på formen $\int \Psi^* (\cdots) \Psi\, dx = \langle \cdots \rangle$:

$$\int (\tilde{A}\Psi)^* \tilde{A}\Psi\, dx = \int \Psi^* \tilde{A}\tilde{A}\Psi\, dx = \langle \tilde{A}^2 \rangle = (\Delta A)^2$$

$$\int (\tilde{B}\Psi)^* \tilde{B}\Psi\, dx = \int \Psi^* \tilde{B}\tilde{B}\Psi\, dx = \langle \tilde{B}^2 \rangle = (\Delta B)^2$$

$$\int (\tilde{A}\Psi)^* \tilde{B}\Psi\, dx - \int (\tilde{B}\Psi)^* \tilde{A}\Psi\, dx = \langle \tilde{A}\tilde{B} \rangle - \langle \tilde{B}\tilde{A} \rangle = \langle [\tilde{A}, \tilde{B}] \rangle$$

Dvs: $(\Delta A)^2 + (\Delta B)^2 \alpha^2 + i\alpha \langle [\tilde{A}, \tilde{B}] \rangle \geq 0$

Her er $[\tilde{A}, \tilde{B}] = (\hat{A} - \langle A \rangle)(\hat{B} - \langle B \rangle) - (\hat{B} - \langle B \rangle)(\hat{A} - \langle A \rangle)$

$$= \hat{A}\hat{B} - \hat{B}\hat{A} = [\hat{A}, \hat{B}]$$

Øvrige ledd kansellerer, fordi de reelle tallene $\langle A \rangle$ og $\langle B \rangle$ kommuterer med $\hat{A}$ og $\hat{B}$.

$$\Rightarrow (\Delta A)^2 + \alpha^2 (\Delta B)^2 + i\alpha \langle [\hat{A}, \hat{B}] \rangle \geq 0 \qquad (\text{alle ledd reelle!})$$

Ganger med $(\Delta B)^2$:

$$(\Delta A)^2(\Delta B)^2 \geq -\alpha^2(\Delta B)^4 - \alpha\langle i[\hat{A},\hat{B}]\rangle(\Delta B)^2$$

Høyre side er parabel med negativ krumning, finner max-verdien:

$$\frac{d}{d\alpha}\left\{-\alpha^2(\Delta B)^4 - \alpha\langle i[\hat{A},\hat{B}]\rangle(\Delta B)^2\right\} = 0 \Rightarrow \alpha = -\frac{\langle i[\hat{A},\hat{B}]\rangle}{2(\Delta B)^2}$$

$$\Rightarrow (\Delta A)^2(\Delta B)^2 \geq \left(-\frac{1}{4}+\frac{1}{2}\right)\langle i[\hat{A},\hat{B}]\rangle^2 = \frac{1}{4}\langle i[\hat{A},\hat{B}]\rangle^2$$

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

Eks 1: $[x,\hat{p}_x] = i\hbar \quad \Rightarrow \quad \Delta x\cdot\Delta p_x \geq \hbar/2$

Eks 2: $[y,\hat{p}_x] = 0 \quad \Rightarrow \quad \Delta y\cdot\Delta p_x \geq 0$

$\Rightarrow$ y og p_x <u>kan</u> måles presist samtidig

Eks 3: Hva slags $\Psi(x)$ gir <u>minimalt</u> uskarphetsprodukt $\Delta x\cdot\Delta p = \hbar/2$?

Løsn: $\tilde{A}\Psi + i\alpha\tilde{B}\Psi = 0$

$$\Rightarrow (x-\langle x\rangle)\Psi + \alpha\hbar\left(\frac{\partial}{\partial x} - \frac{i\langle p\rangle}{\hbar}\right)\Psi = 0$$

$$\Rightarrow \frac{\partial\Psi}{\Psi} = \left[-\frac{x-\langle x\rangle}{\alpha\hbar} + \frac{i\langle p\rangle}{\hbar}\right]\partial x$$

$$\Rightarrow \Psi(x) \sim \exp\left[-\frac{(x-\langle x\rangle)^2}{2\alpha\hbar} + \frac{i\langle p\rangle x}{\hbar}\right]$$

$$\text{med } 2\alpha\hbar = 2\cdot\underbrace{\left(-\frac{i\langle[x,\hat{p}]\rangle}{2(\Delta p)^2}\right)}_{\alpha}\cdot\underbrace{2\Delta x\Delta p}_{\hbar} = 2\cdot\frac{2\Delta x\Delta p}{2(\Delta p)^2}\cdot 2\Delta x\Delta p$$

$$= (2\Delta x)^2$$

$$\Rightarrow \Psi(x) \sim \exp\left[-\left(\frac{x-\langle x\rangle}{2\Delta x}\right)^2 + i\frac{\langle p\rangle}{\hbar}x\right]$$

Som er en <u>gaussisk bølgepakke</u>. [Øv. 2]

Tidsutvikling av forventningsverdier

[PCH 4.3 ; DJG 3.4.3 ; IØ 4.3]

$$\frac{d}{dt}\langle F\rangle = \frac{d}{dt}\left\{\int \Psi^* \hat{F}\, \Psi\, dx\right\}$$

$$= \int \frac{\partial \Psi^*}{\partial t}\hat{F}\,\Psi\, dx + \int \Psi^* \hat{F}\frac{\partial \Psi}{\partial t}\, dx + \int \Psi^* \frac{\partial \hat{F}}{\partial t}\Psi\, dx$$

Hermitesk!

$$= \int \left(\frac{\hat{H}\Psi}{i\hbar}\right)^* \hat{F}\,\Psi\, dx + \int \Psi^* \hat{F}\left(\frac{\hat{H}\Psi}{i\hbar}\right) dx + \left\langle \frac{\partial \hat{F}}{\partial t}\right\rangle$$

$$= \frac{i}{\hbar}\int \Psi^* \hat{H}\hat{F}\,\Psi\, dx - \frac{i}{\hbar}\int \Psi^* \hat{F}\hat{H}\,\Psi\, dx + \left\langle \frac{\partial \hat{F}}{\partial t}\right\rangle$$

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

Ofte er $\hat{F}$ uavh. av t, dvs $\partial\hat{F}/\partial t = 0$. Da er:

$$\frac{d}{dt}\langle F\rangle = \frac{i}{\hbar}\langle [\hat{H},\hat{F}]\rangle$$

Dermed, hvis $\hat{F}$ kommuterer med $\hat{H}$, er $\langle F\rangle$ en bevegelseskonstant.

Eks: Fri partikkel.

$$\hat{H} = \hat{p}^2/2m$$

$$\Rightarrow [\hat{H},\hat{p}] = \frac{1}{2m}(\hat{p}^3 - \hat{p}^3) = 0$$

$$\Rightarrow \langle p\rangle = \text{konstant}$$

Som ventet; ingen krefter på partikkelen.

Ehrenfests teorem

[PCH 4.4 ; DJG 1.5, 4.1 ; IØ 4.4]

Kvantemekaniske middelverdier oppfyller klassiske bevegelsesligninger : (Newton: $\vec{F} = d\vec{p}/dt = -\nabla V$)

$$\boxed{\begin{array}{lll} \text{1D:} & \frac{d}{dt}\langle x\rangle = \frac{\langle p\rangle}{m}, & \frac{d}{dt}\langle p\rangle = \left\langle -\frac{\partial V}{\partial x}\right\rangle \\ \text{3D:} & \frac{d}{dt}\langle \vec{r}\rangle = \frac{\langle \vec{p}\rangle}{m}, & \frac{d}{dt}\langle \vec{p}\rangle = \langle -\nabla V\rangle \end{array}}$$

Bevis (i 1D): $\hat{H} = \hat{p}^2/2m + V(x,t)$

$$\Rightarrow \frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle[\hat{H},x]\rangle = \frac{i}{2m\hbar}\langle[\hat{p}^2,x]\rangle \qquad ([V,x]=0)$$

$$[\hat{p}^2,x] = \hat{p}\hat{p} - x\hat{p}\hat{p} = \hat{p}\hat{p}x - \hat{p}x\hat{p} + \hat{p}x\hat{p} - x\hat{p}\hat{p}$$

$$= \hat{p}[\hat{p},x] + [\hat{p},x]\hat{p} = -2i\hbar\hat{p}$$

$$\Rightarrow \frac{d}{dt}\langle x\rangle = \frac{i}{2m\hbar}\cdot(-2i\hbar)\cdot\langle\hat{p}\rangle = \underline{\frac{\langle p\rangle}{m}}$$

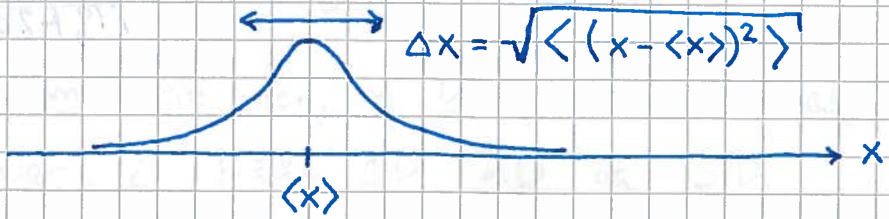
$$\frac{d}{dt}\langle p\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{p}]\rangle = \frac{i}{\hbar}\langle[V,\hat{p}]\rangle \qquad ([\hat{K},\hat{p}]=0)$$

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

$$\Rightarrow \frac{d}{dt}\langle p\rangle = \frac{i}{\hbar}\cdot\left(-\frac{\hbar}{i}\right)\cdot\left\langle\frac{\partial V}{\partial x}\right\rangle = \left\langle -\frac{\partial V}{\partial x}\right\rangle,$$ Newtons 2. lov!

qed

Anta partikkel beskrevet med en bølgepakke:



$$\frac{d\langle p \rangle}{dt} = m \frac{d^2 \langle x \rangle}{dt^2} = \langle F(x) \rangle \quad ; \quad \text{kraft } F(x) = -\frac{\partial V}{\partial x}$$

$\Rightarrow$ $\langle x \rangle$ følger den klassiske banen dersom $\langle F(x) \rangle = F(\langle x \rangle)$

Rekkeutvikler F omkring $\langle x \rangle$:

$$F(x) = F(\langle x \rangle) + (x - \langle x \rangle) F'(\langle x \rangle) + \frac{1}{2}(x - \langle x \rangle)^2 F''(\langle x \rangle) + \ldots$$

$$\Rightarrow \quad \langle F(x) \rangle = F(\langle x \rangle) + \frac{1}{2}(\Delta x)^2 F''(\langle x \rangle) + \ldots$$

$\Rightarrow$ Ser at Newton-mekanikk holder, dvs $\langle F(x) \rangle \approx F(\langle x \rangle)$, dersom

- Δx kan neglisjeres (makroskopiske partikler)

og/eller
- $F''(\langle x \rangle)$, $F'''(\langle x \rangle)$ ... kan neglisjeres (langsomt varierende $V(x)$)

Eks: Harmonisk oscillator

$$V(x) \sim x^2 \quad \Rightarrow \quad F'' = F''' = \ldots = 0 \quad \Rightarrow \quad \langle F(x) \rangle = F(\langle x \rangle)$$

$\Rightarrow$ Bølgepakke vil svinge fram og tilbake som en masse festet til ideell fjær.

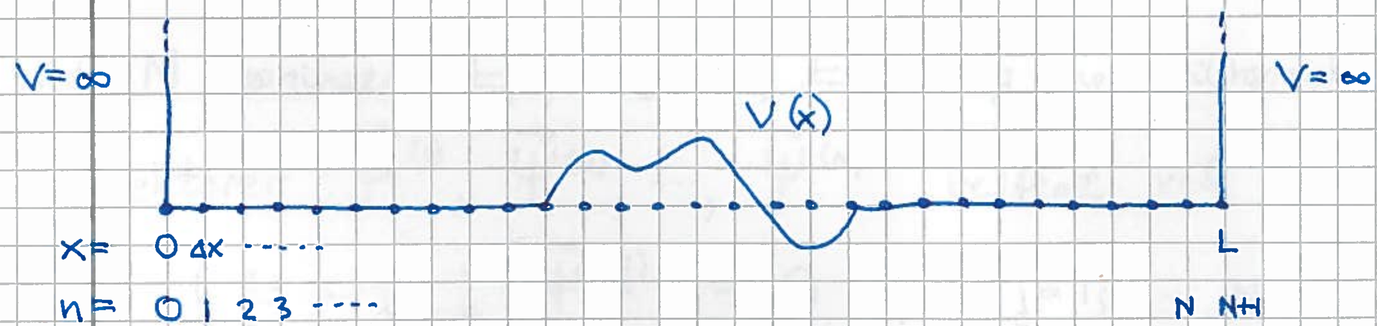
Enkel numerisk løsning av TUSL

Vi skal motivere for, og løse, noen analytisk løsbare potensialer, i både 1D, 2D og 3D.

Men først ser vi på en enkel oppskrift på numerisk løsning i 1D.

TUSL : $-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x)$

Strategi: Diskretiser området $0 < x < L$ slik at det interessante intervallet for $V(x)$ er langt unna $x=0$ og $x=L$. Sett $V=\infty$ for $x \le 0$ og $x \ge L$.



$$\Rightarrow \quad x_n = n\cdot\Delta x, \quad V_n = V(x_n) = V(n\cdot\Delta x), \quad \psi_n = \psi(x_n) = \psi(n\cdot\Delta x)$$

$$V_0 = V_{N+1} = \infty \quad \Rightarrow \quad \psi_0 = \psi_{N+1} = 0$$

$$\psi_n'' \approx \frac{\psi'_{n+1/2} - \psi'_{n-1/2}}{\Delta x} \approx \frac{(\psi_{n+1}-\psi_n)/\Delta x - (\psi_n - \psi_{n-1})/\Delta x}{\Delta x}$$

$$= \frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{(\Delta x)^2}$$

TUSL blir nå et sett av N differanseligninger:

$$-\frac{\hbar^2}{2m\,\Delta x^2}\,\psi_{n-1} + \left(\frac{\hbar^2}{m\,\Delta x^2} + V_n\right)\psi_n - \frac{\hbar^2}{2m\,\Delta x^2}\,\psi_{n+1} = E\,\psi_n$$

$(n = 1, 2, ---, N)$

dvs $\mathbb{H}\,\vec{\psi} = E\,\vec{\psi}$, med tridiagonal matrise $\mathbb{H}$

med elementer $H_{nn} = \frac{\hbar^2}{m\,\Delta x^2} + V_n$, $H_{n,n\pm 1} = -\frac{\hbar^2}{2m\,\Delta x^2}$,

$H_{ij} = 0$ ellers. Dvs, $\mathbb{H}$ er reell, symmetrisk, $N \times N$.

Ikke-trivielle løsninger, dvs $\vec{\psi} \neq 0$, bare når

$\det(\mathbb{H} - E\,\mathbb{I}) = 0$, som gir en N-te-gradsligning

$$c_N E^N + c_{N-1} E^{N-1} + \dots + c_1 E + c_0 = 0$$

med N løsninger $E_1, E_2, ---, E_N$, og med tilhørende

egenvektorer $\vec{\psi}^{(1)}, \vec{\psi}^{(2)}, ---, \vec{\psi}^{(N)}$ bestemt ved

$$(\mathbb{H} - E_j\,\mathbb{I})\,\vec{\psi}^{(j)} = 0 \; ; \quad j = 1, 2, --, N$$

Normering: $\sum_{n=1}^{N} |\psi_n^{(j)}|^2 \,\Delta x = 1$

(Dvs, $\psi_n^{(j)} = \psi^{(j)}(x_n)$ = verdien av $\psi^{(j)}$ i posisjon $x_n = n \cdot \Delta x$)

Python:

```
import numpy as np
w, v = np.linalg.eigh(H)
```

$\Rightarrow$ $w[0] = E_1$, ---, $w[N-1] = E_N$

$v[n-1, j-1] = \psi_n^{(j)}$

Matlab:

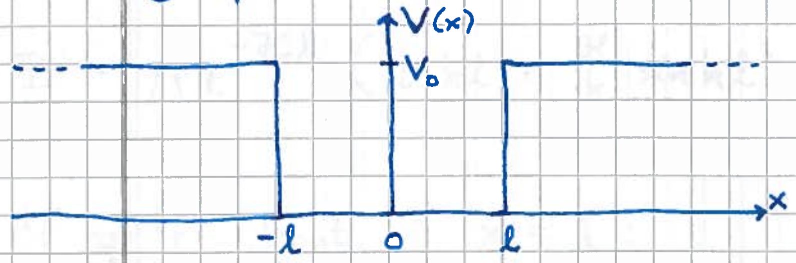
```
[v,w] = eig(H)
```

$\Rightarrow$ $w(1,1) = E_1$, ---, $w(N,N) = E_N$

$v(n,j) = \psi_n^{(j)}$

Endelig potensialbrønn

[PCH 3.3 ; DJG 2.6 ; IØ 3.2]



Relevans:

Halvlederteknologi

$$V(x) = \begin{cases} 0 & ; \ |x| < \ell \\ V_0 & ; \ |x| > \ell \end{cases} \Rightarrow \text{TUSL}: \quad \psi''(x) = \begin{cases} -\dfrac{2mE}{\hbar^2}\psi(x) & ; \ |x| < \ell \\ \dfrac{2m(V_0 - E)}{\hbar^2}\psi(x) & ; \ |x| > \ell \end{cases}$$

$E < V_0$: Bundne tilstander

$$\psi(x) = C \sin kx + D \cos kx \quad ; \quad k = \frac{\sqrt{2mE}}{\hbar} \quad ; \quad |x| < \ell$$

$$\psi(x) = A e^{\varkappa x} + B e^{-\varkappa x} \quad ; \quad \varkappa = \sqrt{2m(V_0 - E)}/\hbar \quad ; \quad |x| > \ell$$

$$e^{\pm \varkappa x} \xrightarrow{x \to \pm\infty} \infty \Rightarrow \psi(x) = \begin{cases} A e^{\varkappa x} & ; \ x < -\ell \\ B e^{-\varkappa x} & ; \ x > \ell \end{cases}$$

De 5 ukjente (A, B, C, D og energien E) fastlegges med normering $\left(\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1\right)$ og fire grensebetingelser (ψ og ψ' kontinuerlige i $x = \pm \ell$).

Symmetrisk $V(x) \Rightarrow$ symm. $|\psi(x)|^2 \Rightarrow$ symm. ($D \cos kx$) og antisymm. ($C \sin kx$) løsninger for $\psi(x)$.

ψ og ψ' kont. i $x = -\ell$:

$$A e^{-\varkappa \ell} = -C \sin k\ell + D \cos k\ell \qquad (1)$$

$$A \varkappa e^{-\varkappa \ell} = k\left(C \cos k\ell + D \sin k\ell\right) \qquad (2)$$

$$(1) \cdot \sin k\ell - (2) \cdot \frac{1}{k} \cos k\ell$$

$$\Rightarrow C = A e^{-\varkappa \ell}\left(\frac{\varkappa}{k} \cos k\ell - \sin k\ell\right) = A e^{-\varkappa \ell} \cos k\ell \left(\frac{\varkappa}{k} - \tan k\ell\right) \quad (3)$$

$(1) \cdot \cos k\ell + (2) \cdot \frac{1}{k} \sin k\ell$

$$\Rightarrow D = A e^{-\varkappa \ell} \left(\cos k\ell + \frac{\varkappa}{k} \sin k\ell \right) = A e^{-\varkappa \ell} \cos k\ell \left(1 + \frac{\varkappa}{k} \tan k\ell \right) \quad (4)$$

ψ og ψ' kont. i $x = \ell$:

$$B e^{-\varkappa \ell} = C \sin k\ell + D \cos k\ell \qquad (5)$$

$$-B\varkappa e^{-\varkappa \ell} = k \left(C \cos k\ell - D \sin k\ell \right) \qquad (6)$$

$(5) \cdot \frac{\varkappa}{k} + (6) \cdot \frac{1}{k}$

$$\Rightarrow C \left(\frac{\varkappa}{k} \sin k\ell + \cos k\ell \right) + D \left(\frac{\varkappa}{k} \cos k\ell - \sin k\ell \right) = 0$$

$$\Rightarrow C \left(\frac{\varkappa}{k} \tan k\ell + 1 \right) + D \left(\frac{\varkappa}{k} - \tan k\ell \right) = 0 \qquad (7)$$

(3) og (4) for hhv C og D inn i (7) gir to like ledd:

$$2 \left(\frac{\varkappa}{k} \tan k\ell + 1 \right) \left(\frac{\varkappa}{k} - \tan k\ell \right) = 0$$

Antisymm. løsn:

$\frac{\varkappa}{k} \tan k\ell + 1 = 0 \Rightarrow D = 0 \Rightarrow \psi(x) = C \sin kx$

Symm. løsn:

$\frac{\varkappa}{k} - \tan k\ell = 0 \Rightarrow C = 0 \Rightarrow \psi(x) = D \cos kx$

Energiegenverdiene E er gitt ved:

$$\tan k\ell = \begin{cases} \varkappa / k & ; \text{ symm.} \quad (S) \\ -k/\varkappa & ; \text{ antisymm.} \quad (AS) \end{cases}$$

$$\Rightarrow \tan \frac{\sqrt{2mE}\,\ell}{\hbar} = \begin{cases} \sqrt{\frac{V_0 - E}{E}} & ; \quad S \\ -\sqrt{\frac{E}{V_0 - E}} & ; \quad AS \end{cases}$$