Normering for ψ_n

Vi har at $\int_{-\infty}^{\infty} \psi^* \hat{a}_{\mp} \psi \, dx = \int_{-\infty}^{\infty} (\hat{a}_{\pm}\psi)^* \psi \, dx$

$$\langle \psi | \hat{a}_{\pm} \psi \rangle = \langle \hat{a}_{\mp} \psi | \psi \rangle$$

Generelt er $\int_{-\infty}^{\infty} \psi^* \hat{Q} \psi \, dx = \int_{-\infty}^{\infty} (\hat{Q}^{\dagger} \psi)^* \psi \, dx$

$$\langle \psi | \hat{Q} \psi \rangle = \langle \hat{Q}^{\dagger} \psi | \psi \rangle$$

hvor $\hat{Q}^{\dagger}$ kalles den <u>hermitisk konjugerte</u> til $\hat{Q}$

Så $\hat{a}_+^{\dagger} = \hat{a}_-$ og $\hat{a}_-^{\dagger} = \hat{a}_+$.

Bevis: $\int_{-\infty}^{\infty} \psi^* \hat{a}_{\pm} \psi \, dx = \frac{1}{\sqrt{2\hbar m\omega}} \int_{-\infty}^{\infty} \psi^* (\mp i \hat{p} + m\omega \hat{x}) \psi \, dx$

$$= \frac{1}{\sqrt{2\hbar m\omega}} \int_{-\infty}^{\infty} \psi^* \left(\mp \hbar \frac{d}{dx} + m\omega x\right) \psi \, dx$$

$$= \frac{1}{\sqrt{2\hbar m\omega}} \left[\cancel{\mp \hbar \psi^* \psi \Big|_{-\infty}^{\infty}} \pm \hbar \int_{-\infty}^{\infty} \left(\frac{d}{dx}\psi^* \psi + \frac{m\omega}{\hbar} x \psi^* \psi \right) dx \right]$$

$$= \frac{1}{\sqrt{2\hbar m\omega}} \int_{-\infty}^{\infty} \left(\pm \hbar \frac{d}{dx} + m\omega x\right) \psi^* \psi \, dx$$

$$= \frac{1}{\sqrt{2\hbar m\omega}} \int_{-\infty}^{\infty} \left[\left(\pm \hbar \frac{d}{dx} + m\omega x\right) \psi \right]^* \psi \, dx$$

$$= \int_{-\infty}^{\infty} (\hat{a}_{\mp} \psi)^* \psi \, dx$$

Anta ψ_n er normalisert. Dvs. $\int_{-\infty}^{\infty} |\psi_n|^2 dx = 1$

Løsningen ψ_{n+1} er gitt som $\psi_{n+1} = A_n \hat{a}_+ \psi_n$. Vil finne A_n.

$$\int_{-\infty}^{\infty} |\psi_{n+1}|^2 dx = \int_{-\infty}^{\infty} |A_n|^2 (\hat{a}_+\psi_n)^* \hat{a}_+\psi_n \, dx = |A_n|^2 \int_{-\infty}^{\infty} (\hat{a}_-\hat{a}_+\psi_n)^* \psi_n \, dx$$

$$\hat{a}_-\hat{a}_+ = \hat{a}_+\hat{a}_- + 1$$

$$\hat{N} = \hat{a}_+\hat{a}_-$$

$$= |A_n|^2 \int_{-\infty}^{\infty} ((\hat{N}+1)\psi_n)^* \psi_n \, dx = |A_n|^2 \int_{-\infty}^{\infty} (n+1)\psi_n^* \psi_n \, dx$$

$$= |A_n|^2 (n+1) = 1$$

$$\Rightarrow A_n = \frac{1}{\sqrt{n+1}}$$

Generelt er da $\boxed{\psi_n = \frac{1}{\sqrt{n!}} \hat{a}_+^n \psi_0}$

$$\hat{a}_-\psi_0 = 0$$

Eksempel: Finn $\int_{-\infty}^{\infty} \psi_2^* \psi_1 \, dx = \int_{-\infty}^{\infty} \Big(\frac{1}{\sqrt{2}} \underbrace{\hat{a}_+\hat{a}_+\psi_0}\Big)^* \hat{a}_+\psi_0 \, dx$

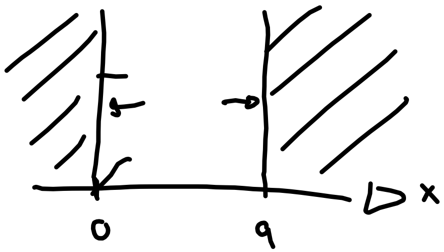
Et eksempel på at

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx = \delta_{mn} = \begin{cases} 1 & \text{når } m=n \\ 0 & \text{ellers} \end{cases}$$

$$= \frac{1}{\sqrt{2}} \int_{-\infty}^{\infty} \psi_0^* \hat{a}_- \underline{\hat{a}_-\hat{a}_+} \psi_0 \, dx = \frac{1}{\sqrt{2}} \int_{-\infty}^{\infty} \psi_0^* \hat{a}_- (1 + \hat{a}_+\hat{a}_-)\psi_0 \, dx$$

$$= \frac{1}{\sqrt{2}} \int_{-\infty}^{\infty} \psi_0^* \underline{\hat{a}_-\psi_0} + \psi_0^* \hat{a}_-\hat{a}_+ \underline{\hat{a}_-\psi_0} \, dx = 0$$

OBS! FARE!



Kvantemekanikk definert på $0 \leq x \leq a$

har ingen grensebetingelser i $x=0$ og $x=a$!

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < a \\ \infty & \text{for } x=0 \text{ og } x=a \end{cases}$$

Analytisk løsning av HO TUSL

TUSL HO: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi$

Dimensjonsløs koordinat $\xi = \sqrt{\frac{m\omega}{\hbar}}\,x$ $[\hbar] = Js = kg\,m^2 s^{-1}$

(xi)

$$\frac{d\xi}{dx} = \sqrt{\frac{m\omega}{\hbar}} \Rightarrow \frac{d^2\psi}{dx^2} = \frac{d^2\psi}{d\xi^2}\frac{m\omega}{\hbar}$$

$\Rightarrow$ TUSL HO
$$-\frac{\hbar^{\cancel{2}}}{2\cancel{m}}\frac{\cancel{m}\omega}{\cancel{\hbar}}\frac{d^2\psi}{d\xi^2} + \frac{1}{2}\cancel{m}\omega^{\cancel{2}}\frac{\hbar}{\cancel{m\omega}}\xi^2\psi = E\psi$$

$$-\frac{1}{2}\hbar\omega\frac{d^2\psi}{d\xi^2} + \frac{1}{2}\hbar\omega\xi^2\psi = E\psi \quad \Big) \cdot \frac{1}{\frac{1}{2}\hbar\omega}$$

$$-\frac{d^2\psi}{d\xi^2} + \xi^2\psi = K\psi \qquad \text{hvor } K = \frac{E}{\frac{1}{2}\hbar\omega}$$

$$\boxed{\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi}$$

Grensebetingelse: $V(x) \xrightarrow{|x|\to\infty} \infty$ slik at $\psi(x) \xrightarrow{|x|\to\infty} 0$

Når $|x|$ ($|\xi|$) blir stor så er $\frac{d^2\psi}{d\xi^2} \simeq \xi^2\psi$

Når $|x|$ ($|\xi|$) blir stor så er $\frac{d^2\psi}{d\xi^2} \simeq \xi^2 \psi$

Denne har løsning $\psi(\xi) = \underline{A e^{-\frac{1}{2}\xi^2}} + \underline{B e^{\frac{1}{2}\xi^2}}$

Må ha $B = 0$ for å oppfylle grensebetingelsen.

Antyder at løsninger av TUSL kan skrives

$$\boxed{\psi(\xi) = h(\xi) e^{-\frac{1}{2}\xi^2}}$$

Hvordan ser ligningen for h ut?

$$\frac{d\psi}{d\xi} = \frac{dh}{d\xi} e^{-\frac{1}{2}\xi^2} - h\xi e^{-\frac{1}{2}\xi^2} = \left(\frac{dh}{d\xi} - \xi h\right) e^{-\frac{1}{2}\xi^2}$$

$$\frac{d^2\psi}{d\xi^2} = \left(\frac{d^2h}{d\xi^2} - h - \xi\frac{dh}{d\xi}\right)e^{-\frac{1}{2}\xi^2} - \left(\frac{dh}{d\xi} - \xi h\right)\xi e^{-\frac{1}{2}\xi^2}$$

$$= \left(\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2 - 1)h\right)e^{-\frac{1}{2}\xi^2}$$

TUSL blir da

$$\boxed{\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2-1)h = (\xi^2 - K)h} \Rightarrow \boxed{\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0}$$

Løsning ved Frobenius metode

Anta $h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$

$$\frac{dh}{d\xi} = \sum_{j=0}^{\infty} \frac{d}{d\xi}(a_j \xi^j) = \sum_{j=0}^{\infty} j a_j \xi^{j-1}, \quad \frac{d^2h}{d\xi^2} = \sum_{j=2}^{\infty} j(j-1) a_j \xi^{j-2} = \sum_{j=0}^{\infty} (j+2)(j+1) a_{j+2} \xi^j$$

TUSL blir

$$\sum_{j=0}^{\infty} (j+2)(j+1) a_{j+2} \xi^j - \sum_{j=0}^{\infty} 2 j a_j \xi^j + \sum_{j=0}^{\infty} (K-1) a_j \xi^j = 0$$

$$\sum_{j=0}^{\infty} \left[(j+2)(j+1) a_{j+2} - 2 j a_j + (K-1) a_j \right] \xi^j = 0$$

$$\Rightarrow (j+2)(j+1) a_{j+2} - 2 j a_j + (K-1) a_j = 0$$

$$\Rightarrow a_{j+2} = \frac{2j - K + 1}{(j+2)(j+1)} a_j$$ rekursjonsformel for a_j

Trenger a_0 og a_1 for å ha hele løsningen.

Husk at $\psi(\xi) = h(\xi) e^{-\frac{1}{2}\xi^2}$. $h(\xi) \xrightarrow{|\xi| \to \infty} \infty$ dersom rekken ikke terminerer.

Når $j \to \infty$ så er $a_{j+2} \simeq \frac{2}{j} a_j = \frac{a_j}{j/2}$ dvs. $a_j \simeq \frac{a_0}{(j/2)!}$ for store j og partalls j

$$\lim_{|\xi|\to\infty} h(\xi) \simeq \sum_{\substack{\text{alle } j\\ \text{partall}}} \frac{a_0}{(j/2)!}\xi^j \simeq a_0 \sum \frac{\xi^{2(j/2)}}{(j/2)!} = \underline{a_0 e^{\frac{1}{2}\xi^2}}$$

Konklusjon: <u>rekken må terminere.</u>

Det må finnes en j_{maks} slik at $a_{j_{maks}+2} = 0$ og $a_0 = 0$ <u>eller</u> $a_1 = 0$

Dette skjer dersom $\underline{2j_{maks} - K + 1 = 0}$. Vi kaller j_{maks} for n.

Vi har da at $K = 2n+1 \Rightarrow \frac{E_n}{\frac{1}{2}\hbar\omega} = 2n+1 \Rightarrow \underline{E_n = \hbar\omega(n+\frac{1}{2})}$