Innføring i kvantemek. I 22.1.81.

Løsninger.

I a $H\Psi = i\hbar \frac{\partial \Psi}{\partial t}$ Stasjonær løsning $\Psi(x,t) = \psi(x)\, e^{-\frac{i}{\hbar}Et}$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi \qquad 0 \le x \le L$$

$$\psi = 0 \qquad x<0 \text{ eller } x>L$$

Generelle løsninger:

$$\psi_n = A \sin k_n x + B \cos k_n x \qquad k_n = \sqrt{\frac{2mE_n}{\hbar^2}}$$

Skjøting ved $x=0$ og $x=L$ gir $B=0$ og $k_n = \frac{\pi}{L}n$:

$$\underline{\underline{\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi}{L} n x \; e^{-\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}n^2 t}}} \qquad E_n = \frac{\hbar^2 k^2}{2m} = \underline{\underline{\frac{\hbar^2\pi^2}{2mL^2}n^2}}$$

når normert $\int_0^L |\psi_n|^2 dx = 1$.

b. Fra løsningen i a) $\underline{\underline{E_1 = \frac{\hbar^2\pi^2}{2mL^2}}}$

i) $$P_\ell = \int_0^\ell |\psi_1|^2 dx = \frac{2}{L}\int_0^\ell \sin^2 \frac{\pi}{L} x \, dx = \frac{2}{\pi}\int_0^{\frac{\pi}{L}\ell} \frac{1-\cos 2y}{2} dy, \qquad y = \frac{\pi}{L}x$$

$$= \underline{\underline{\frac{\ell}{L} - \frac{1}{2\pi}\sin 2\pi \frac{\ell}{L}}}$$

ii) Som i a) bare med $L \to \ell$:

$$\underline{\phi_n = \begin{cases} \sqrt{\frac{2}{\ell}} \sin \frac{\pi}{\ell} n x & 0 \le x \le \ell \\ 0 & \text{ellers.} \end{cases}} \qquad \underline{E_n^\ell = \frac{\pi^2\hbar^2}{2m\ell^2}n^2}$$

iii) $$\Psi(x,t) = \sum_{n=1}^\infty c_n \Phi_n(x,t) \qquad \Phi_n(x,t) = \phi_n(x)\, e^{-\frac{i}{\hbar}E_n^\ell t}, \quad c_n = \text{konstant}$$

ved $t=0$

$$c_n = \int_0^\ell \phi_n^*(x)\, \Psi_L(x,0)\, dx = \frac{2}{\sqrt{\ell L}}\int_0^\ell \sin \frac{\pi}{\ell}nx \, \sin \frac{\pi}{L}x \, dx$$

$$= \frac{2}{\sqrt{\ell L}}\frac{1}{2}\int_0^\ell \left[\cos \pi\left(\frac{n}{\ell} - \frac{1}{L}\right)x - \cos \pi\left(\frac{n}{\ell}+\frac{1}{L}\right)x\right] dx$$

$$= \frac{\sqrt{\ell L}}{\pi}\left[\frac{1}{nL-\ell}\sin \pi\left(n - \frac{\ell}{L}\right) - \frac{1}{nL+\ell}\sin \pi\left(n+\frac{\ell}{L}\right)\right]$$

$$= \underline{\frac{1}{\pi}\sqrt{\frac{\ell}{L}}\frac{2n}{n^2-\left(\frac{\ell}{L}\right)^2}(-1)^{n+1}\sin \pi \frac{\ell}{L}}$$

$$\underline{\underline{P_n = |c_n|^2 = \frac{4}{\pi^2}\frac{\ell}{L}\frac{n^2}{\left[n^2-\left(\frac{\ell}{L}\right)^2\right]^2}\sin^2 \pi \frac{\ell}{L}}}$$

innf. kv. mek. 22.1.81

Løsning. forts.

I b) iv) For $l = \frac{1}{2}L$; $C_n = \frac{1}{\pi}\sqrt{\frac{1}{2}}\,(-1)^{n+1}\frac{2n}{n^2-\frac{1}{4}}\sin\frac{\pi}{2} = \frac{\sqrt{2}}{\pi}(-1)^{n+1}\frac{4n}{4n^2-1}$

gir
$$\Psi(x,t) = \sum_{n=1}^{\infty}(-1)^{n+1}\frac{8}{\pi}\sqrt{\frac{2}{L}}\,\frac{n}{4n^2-1}\sin\frac{2\pi}{L}n\,x\; e^{-i\frac{2\pi^2\hbar}{mL^2}n^2 t}$$

Rekurenstid $T = \frac{4ml^2}{\pi\hbar}N$ N = helt tall $\Psi(x, t = \frac{4ml^2}{\pi\hbar}N) = \Psi(x, t=0)$

II a) Gitt $[A,B] = 0$ og $A\psi_n = a_n\psi_n$ $n = 1, 2, 3 \dots$

Da er $A(B\psi_n) = BA\psi_n = a_n(B\psi_n)$

Altså $B\psi_n$ er egenf. til A med egenverdi a_n og da det her ikke er noen degenerasjon må

$$\underline{B\psi_n = b_n\psi_n} \quad \text{for alle } n.$$

b) Fri partikkel

Energi operator $H = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$

Impuls op. $\vec{p} = \{p_x, p_y, p_z\} = \left\{\frac{\hbar}{i}\frac{\partial}{\partial x}, \frac{\hbar}{i}\frac{\partial}{\partial y}, \frac{\hbar}{i}\frac{\partial}{\partial z}\right\}$

Paritets op. $\mathbb{P}\,\psi(\vec{r}) = \psi(-\vec{r})$

Kommutatorene:

$$[p_x, H] = -\frac{\hbar^2}{2m}\frac{\hbar}{i}\left(\left[\frac{\partial}{\partial x}, \frac{\partial^2}{\partial x^2}\right] + \left[\frac{\partial}{\partial x}, \frac{\partial^2}{\partial y^2}\right] + \left[\frac{\partial}{\partial x}, \frac{\partial^2}{\partial z^2}\right]\right) = 0$$

$$[\mathbb{P}, H]\psi(\vec{r}) = -\frac{\hbar^2}{2m}\left[\left(\frac{\partial^2}{\partial(-x)^2} + \frac{\partial^2}{\partial(-y)^2} + \frac{\partial^2}{\partial(-z)^2}\right)\psi(-\vec{r}) - \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(-\vec{r})\right] = 0$$

$$[\mathbb{P}, p_x]\psi(\vec{r}) = \frac{\hbar}{i}\left(\frac{\partial}{\partial(-x)}\psi(-\vec{r}) - \frac{\partial}{\partial x}\psi(-\vec{r})\right) = \underline{-\frac{2\hbar}{i}\frac{\partial}{\partial x}\psi(-\vec{r}) \neq 0} \quad \text{for noen } \psi(\vec{r})$$

Felles egenf. for $\vec{p}$ og H:

Egenf. for H: $-\frac{\hbar^2}{2m}\nabla^2\psi_n = E_n\psi_n$ $\quad \psi_n = A_n e^{\frac{i}{\hbar}\vec{p}_n\vec{r}} + B_n e^{-\frac{i}{\hbar}\vec{p}_n\vec{r}}$ $\quad E_n = \frac{p_n^2}{2m}$

Skal være egenf. for $\vec{p}$:

$\vec{p}\psi_n = \frac{\hbar}{i}\nabla\left(A_n e^{\frac{i}{\hbar}\vec{p}_n\vec{r}} + B_n e^{-\frac{i}{\hbar}\vec{p}_n\vec{r}}\right) = \vec{p}_n A_n e^{\frac{i}{\hbar}\vec{p}_n\vec{r}} - \vec{p}_n B_n e^{-\frac{i}{\hbar}\vec{p}_n\vec{r}}$ Egenf. hvis $A_n = 0$ eller $B_n = 0$.

Felles egenf. $\underline{\psi_n^{(H,\vec{p})} = A_n e^{\frac{i}{\hbar}\vec{p}_n\vec{r}}}$ med egenverdier $E_n = \frac{p_n^2}{2m}$ $\quad p_n = \pm\sqrt{2mE_n}\,\hat{e}_p$

For H og $\mathbb{P}$ $\quad \mathbb{P}$ har egenverdiene ± 1

H's egenf. må være egenf. for $\mathbb{P}$ også:

$$\mathbb{P}\psi_n = A_n e^{-\frac{i}{\hbar}\vec{p}_n\vec{r}} + B_n e^{\frac{i}{\hbar}\vec{p}_n\vec{r}} = \pm\left(A_n e^{\frac{i}{\hbar}\vec{p}_n\vec{r}} + B_n e^{-\frac{i}{\hbar}\vec{p}_n\vec{r}}\right) = p\,\psi_n$$

Oppfylt hvis $B_n = \pm A_n$

$$\psi_{n,\pm}^{(H,P)} = \begin{cases} A_n \sin k_n r & p = -1 \\ B_n \cos k_n r & p = +1 \end{cases} \qquad E_n = \frac{\hbar^2 k_n^2}{2m}$$

Intet felles sett for $\vec{p}$ og $\mathbb{P}$.

Innf. kv. mek. 22.1.81

Løsn., forts.

II c Uskarphet $(\Delta A)^2 = \langle (A - \langle A\rangle)^2\rangle$

Med $f = (A - \langle A\rangle)\psi$ og $g = (B - \langle B\rangle)\psi$

hvor A og B er hermiteske operatorer

gir Schwartz ulikhet

$$(\Delta A)^2(\Delta B)^2 = \langle (A - \langle A\rangle)^2\rangle \langle (B - \langle B\rangle)^2\rangle = \int \psi^* (A - \langle A\rangle)^2 \psi\, dq \cdot \int \psi^* (B - \langle B\rangle)^2 \psi\, dq$$

$$= \int \big((A - \langle A\rangle)\psi\big)^* (A - \langle A\rangle)\psi\, dq \cdot \int \big((B - \langle B\rangle)\psi\big)^* (B - \langle B\rangle)\psi\, dq$$

$$= \int |(A - \langle A\rangle)\psi|^2 dq \int |(B - \langle B\rangle)\psi|^2 dq$$

$$\geq \left| \int \big((A - \langle A\rangle)\psi\big)^* (B - \langle B\rangle)\psi\, dq \right|^2 = \left| \int \psi^* (A - \langle A\rangle)(B - \langle B\rangle)\psi\, dq \right|^2$$

$$= \left| \frac{1}{2} \int \psi^* \Big[(A - \langle A\rangle)(B - \langle B\rangle) - (B - \langle B\rangle)(A - \langle A\rangle) + (A - \langle A\rangle)(B - \langle B\rangle) + (B - \langle B\rangle)(A - \langle A\rangle)\Big]\psi\, dq \right|^2$$

$$= \left| \frac{1}{2} \int \psi^* [A, B] \psi\, dq + \int \psi^* \big(\{A, B\}_+ - 2\langle A\rangle\langle B\rangle\big)\psi\, dq \right|^2$$

$$= \frac{1}{4}\Big\{ |\langle [A,B]\rangle|^2 + |\langle \{A,B\}_+ - 2\langle A\rangle\langle B\rangle\rangle|^2 \Big\}$$

da $[A,B]$ er antihermitesk og har imaginære egenverdier mens $\{A,B\}_+ - 2\langle A\rangle\langle B\rangle$ er hermitesk og har reelle egenverdier.

$$(\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} |\langle [A,B]\rangle|^2$$

Altså:

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

III a) $|\psi\rangle = \sum_n c_n |n\rangle$ når $|n\rangle$ fullstendig sett: $\sum_n |n\rangle\langle n| = 1$

Utviklingskoeff.:

$$\langle n|\psi\rangle = \sum_{n'} c_{n'} \langle n|n'\rangle = \sum_{n'} c_{n'} \delta_{nn'} = c_n$$

b) $H'_{n'n} = \langle n'|H|n\rangle = \langle n'|E_n|n\rangle = E_n \langle n'|n\rangle = E_n \delta_{nn'}$ når $H|n\rangle = E_n|n\rangle$

$$H'_{n'n} = \langle n'|H|n\rangle = \sum_{k,k'} \langle n'|k\rangle\langle k|H|k'\rangle\langle k'|n\rangle = S'_{n'k} H_{kk'} S_{k'n}$$ med $S_{k'n} = \langle k'|n\rangle$ og $S'_{n'k} = \langle n'|k\rangle$

Har $\sum_k S'_{n'k} S_{kn} = \sum_k \langle n'|k\rangle\langle k|n\rangle = \langle n'|n\rangle = \delta_{n'n}$ Altså: $S' = S^{-1}$

og dermed for matrisene $H' = S^{-1} H S$

c) $H_0 = M\sigma_z = M\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} M & 0 \\ 0 & -M \end{pmatrix}$ Er på diagonal form i denne repres. og H_0's egenverdier er $\pm M$

$$H = M\sigma_z + J\sigma_x = \begin{pmatrix} M & J \\ J & -M \end{pmatrix}$$

Kan diagonaliseres og egenverdiene finnes fra sekulærdeterminanten

$$\begin{vmatrix} M-\lambda & J \\ J & -M-\lambda \end{vmatrix} = 0 \Rightarrow -(M-\lambda)(M+\lambda) - J^2 = 0 \Rightarrow \lambda^2 - M^2 - J^2 = 0$$

$$\lambda = \pm\sqrt{M^2 + J^2} = \pm M\sqrt{1 + \left(\frac{J}{M}\right)^2}$$