KVANTROV 3

Anders

IV 2

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z)=E\psi(x,y,z)$$

Visa att $\psi(x,y,z)=Ae^{iK\cdot r}=Ae^{i(k_x x+k_y y+k_z z)}$ är en lösn.

Först: Insättn. i S.E. ger:

$$-\frac{\hbar^2}{2m}\left(-k_x^2-k_y^2-k_z^2\right)Ae^{iK\cdot r}=EAe^{iK\cdot r}$$

$$\Leftrightarrow \frac{\hbar^2}{2m}|K|^2\psi=E\psi$$

dvs OK m. energiegenvärdet $E=\frac{\hbar^2|K|^2}{2m}$

Sedan: Lös istället m.h.a. variabelseparation:

$\cancel{\psi(x,y,z)=\psi_x(x,y,z}$ Ansats:

$$\psi(x,y,z)=\psi_x(x)\psi_y(y)\psi_z(z)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2}+\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}+\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}\right)=E$$

$\left\{\frac{\partial}{\partial x}\psi_x\psi_y\psi_z=\frac{\partial\psi_x}{\partial x}\psi_y\psi_z \text{ osv. Dela sedan m. } \psi=\psi_x\psi_y\psi_z\right\}$

$$\Leftrightarrow -\frac{\hbar^2}{2m}\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2}-E=\frac{\hbar^2}{2m}\left(\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}+\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}\right)=-\mu \quad \text{(konst.)}$$

$$\Rightarrow \begin{cases} -\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2}=(E-\mu)\psi_x \Rightarrow \psi_x(x)=A_x e^{ik_x x}+B_x e^{-ik_x x} \\ -\frac{\hbar^2}{2m}\left(\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}+\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}\right)=\mu \end{cases}$$

(där $k_x=\frac{\sqrt{2m(E-\mu)}}{\hbar}$)

P.s.s. $-\frac{\hbar^2}{2m}\frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2}-\mu=\frac{\hbar^2}{2m}\frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2}=-\gamma$ (konst.)

$\Rightarrow \ldots$

$$\ldots \Rightarrow \begin{cases} -\frac{\hbar^2}{2m}\frac{\partial^2 \psi_y}{\partial y^2} = (\mu-\gamma)\psi_y \Rightarrow \psi_y(y) = A_y e^{ik_y y} + B_y e^{-ik_y y} \\ -\frac{\hbar^2}{2m}\frac{\partial^2 \psi_z}{\partial z^2} = \gamma\psi_z \Rightarrow \psi_z(z) = A_z e^{ik_z z} + B_z e^{-ik_z z}, \end{cases}$$

där $k_y = \frac{\sqrt{2m(\mu-\gamma)}}{\hbar}$ och $k_z = \frac{\sqrt{2m\gamma}}{\hbar}$

För att kolla med ursprungliga ekv., sätt $B_i = 0$

$$\Rightarrow \psi = \psi_x\psi_y\psi_z = A_x e^{ik_x x} A_y e^{ik_y y} A_z e^{ik_z z} = \left\{ \begin{array}{l} A_x A_y A_z = A \\ K = (k_x, k_y, k_z) \\ r = (x, y, z) \end{array} \right\} =$$

$$= A e^{iK\cdot r}$$

$$|K|^2 = k_x^2 + k_y^2 + k_z^2 = \frac{2m(E-\mu)}{\hbar^2} + \frac{2m(\mu-\gamma)}{\hbar^2} + \frac{2m\gamma}{\hbar^2} =$$

$$= \frac{2m}{\hbar^2}(E-\mu+\mu-\gamma+\gamma) = \frac{2mE}{\hbar^2} \Leftrightarrow E = \frac{\hbar^2|K|^2}{2m}$$

Tidsberoende

$$-\frac{\hbar^2}{2m}\nabla^2\psi = i\hbar\frac{\partial}{\partial t}\psi$$

variabelsep.:
Sätt $\psi(x,y,z,t) = u(x,y,z)v(t)$ och dela med $\psi = uv$. Detta förfarande funkar när potentialen är tidsoberoende. Här är $V=0$.

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{u}\nabla^2 u = \frac{i\hbar}{v}\frac{\partial v}{\partial t} = \text{konst.} = E$$

tidsob. pot.

$\underline{\underline{u}}$: Samma som tidsoberoende S.E. (redan löst)

$\underline{\underline{v}}$: $v(t) = e^{-\frac{i}{\hbar}E\cdot t} = e^{-i\hbar|K|^2 t/2m}$

$$\Rightarrow \psi = uv = A e^{iK\cdot r - i\frac{\hbar|K|^2}{2m}t}$$

IV 3

$V(x) = \frac{1}{2}kx^2 \quad (k = \text{konst.})$

[illegible]

Ställ upp TOSE. Visa att $\psi(x) = Ae^{-\sqrt{km}\,x^2/2\hbar}$ är OK.
Bestäm energiegenvärdet.

S.E. (inkl. potential): $\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2\right)\psi(x) = E\psi(x)$

Sätt in $\psi(x) = Ae^{-\sqrt{km}\,x^2/2\hbar}$;

$$\frac{\partial\psi}{\partial x} = A\,2x\left(-\frac{\sqrt{km}}{2\hbar}\right)e^{-\sqrt{km}\,x^2/2\hbar} = -x\frac{\sqrt{km}}{\hbar}\psi(x)$$

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2} = -\frac{\sqrt{km}}{\hbar}\psi(x) + x^2\frac{km}{\hbar^2}\psi(x)$$

$$\Rightarrow \binom{\text{V.L.}}{\text{S.E.}}: -\frac{\hbar^2}{2m}\left(-\frac{\sqrt{km}}{\hbar} + x^2\frac{km}{\hbar^2}\right)\psi + \frac{1}{2}kx^2\psi =$$

$$= \left(\frac{\hbar}{2}\sqrt{\frac{k}{m}} - \frac{1}{2}kx^2 + \frac{1}{2}kx^2\right)\psi = \frac{\hbar}{2}\sqrt{\frac{k}{m}}\psi$$

$\binom{\text{H.L.}}{\text{S.E.}}: E\psi \qquad$ Alltså: Lösning OK, med egenv. $E = \frac{\hbar}{2}\sqrt{\frac{k}{m}}$

S.E.: $H\psi = E\psi$, $\quad H$: operator, ψ: egenfunktion, E: egenvärde

IV 5

[fyra fem]

väntar med.

Kvantmekanisk kontinuitetsekvation:

$\frac{\partial P}{\partial t} + \nabla J = 0$, där $P(x,t) = |\psi(x,t)|^2 =$ sannolikhetstäthet

$J(x,t) = -\frac{i\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) =$

$=$ sannolikhetsströmtäthet

Här är $\psi(x,t) = Ae^{i(kx-\omega t)} \Rightarrow \psi^*(x,t) = Ae^{-i(kx-\omega t)}$

$\Rightarrow \psi'(x) = ik\psi(x)$, $\quad (\psi^*)'(x) = -ik\psi^*(x)$

$$J \equiv -\frac{i\hbar}{2m}\left(\psi^*\psi' - \psi(\psi^*)'\right) = -\frac{i\hbar}{2m}\left(\psi^* ik\psi + \psi ik\psi^*\right) =$$

$$= -\frac{i\hbar(ik)}{2m}2|\psi|^2 = +\frac{\hbar k}{m}|A|^2 = \left\{\begin{matrix} v = \frac{p}{m} \\ = \frac{\hbar k}{m}\end{matrix}\right\} = v|A|^2$$

V.S.V.

$$\ldots \quad \hat{H} = \left(\frac{1}{2} + a^{+}a\right)\hbar\omega$$

$$\Rightarrow \hat{H}(a^{+}\psi_n) = \hbar\omega\left(\frac{1}{2} + a^{+}a\right)a^{+}\psi_n = \hbar\omega\left(\frac{a^{+}}{2} + a^{+}a\,a^{+}\right)\psi_n =$$

$$\overset{(*)}{=} \hbar\omega\left(\frac{a^{+}}{2} + a^{+}(1 + a^{+}a)\right)\psi_n = a^{+}\,\hbar\omega\left(\frac{1}{2} + 1 + a^{+}a\right)\psi_n =$$

$$= (\hat{H} + \hbar\omega)\,a^{+}\psi_n = (E_n + \hbar\omega)\,a^{+}\psi_n$$

och:

$$\hat{H}(a\psi_n) = \hbar\omega\left(\frac{1}{2} + a^{+}a\right)a\psi_n = \hbar\omega\left(\frac{1}{2} + aa^{+} - 1\right)a\psi_n =$$

$$= \hbar\omega\left(\frac{a}{2} + a\,a^{+}a - a\right)\psi_n = a\left[\hbar\omega\left(\frac{1}{2} + a^{+}a - 1\right)\right]\psi_n =$$

$$= (\hat{H} - \hbar\omega)\,a\psi_n = (E_n - \hbar\omega)\,a\psi_n$$

OK!

... a) $n=1: \quad P(0<x<\frac{L}{3}) = \frac{1}{3} - \frac{\sin\left(\frac{2\pi}{3}\right)}{2\pi} = \frac{1}{3} - \frac{\sqrt{3}/2}{2\pi} = 0{,}196$

b) $n=2: \quad P(0<x<\frac{L}{3}) = \frac{1}{3} - \frac{\sin\left(4\pi/3\right)}{4\pi} = \frac{1}{3} + \frac{\sqrt{3}/2}{4\pi} = 0{,}402$

c) $n\to\infty: \quad P(0<x<\frac{L}{3}) \to \frac{1}{3} - 0 = \frac{1}{3}$

d) klassiskt: $P(0<x<\frac{L}{3}) = \frac{1}{3}$ (samma slh. överallt)

IV 9 Från IV 11: $E_n = \frac{\pi^2 n^2 \hbar^2}{2mL^2}$

$\hbar = 1{,}055\cdot10^{-34}$ Js

i) elektron, $L = 4$ Å, $m = 9{,}1\cdot10^{-31}$ kg

ii) "damm", $L = 4$ cm, $m = 9{,}1\cdot10^{-6}$ kg

i): $E_n^{i} = n^2\left(\frac{\pi^2\hbar^2}{2mL^2}\right) = n^2(3{,}77\cdot10^{-19})\,\text{J} = n^2(2{,}35)\,\text{eV}$

ii) $E_n^{ii} = n^2\left(\frac{\pi^2\hbar^2}{2mL^2}\right) = n^2(3{,}77\cdot10^{-60})\,\text{J} = n^2(2{,}35\cdot10^{-41})\,\text{eV}$

tillst. m. $E<40$ eV: i) $\sqrt{\frac{40}{2{,}35}} = 4 \quad (E_4^{i} = 37{,}6\text{ eV})$

ii) $\sqrt{\frac{40}{2{,}35\cdot10^{-41}}} = 10^{21}$

kvant → klassisk ⇒ kvantiserat → kontinuerligt

IV 14 $\Phi(x) = \begin{cases} 0 & x\le 0 \\ Nx(x-a) & 0\le x\le a \\ 0 & x>a \end{cases}$ Bestäm N & $\langle x^{-2}\rangle$

vänta med!

$1 = \int_{-\infty}^{\infty} dx\,|\Phi(x)|^2 = \int_0^a N^2x^2(x-a)^2dx = N^2\int_0^a(x^4+x^2a^2-2x^3a)dx =$

$= N^2\left[\frac{x^5}{5}+\frac{a^2x^3}{3}-\frac{x^4a}{2}\right]_0^a = N^2\left(\frac{a^5}{5}+\frac{a^5}{3}-\frac{a^5}{2}\right) = a^5N^2\left(\frac{6+10-15}{30}\right) = \frac{a^5N^2}{30}$

$\Leftrightarrow N = \sqrt{\frac{30}{a^5}}$

...

$$\ldots \langle x^{-2}\rangle = \int_{-\infty}^{\infty} dx\, |\Phi(x)|^2 x^{-2} = \frac{30}{a^5}\int_0^a \frac{x^2}{x^2}(x-a)^2 dx = \frac{30}{a^5}\left[\frac{x^3}{3} - x^2 a + a^2 x\right]_0^a =$$

$$= \frac{30}{a^5}\left(\frac{a^3}{3} - a^3 + a^3\right) = \frac{10}{a^2}$$

(Kom ihåg: Väntevärde $\langle f\rangle = \langle\Psi|f|\Psi\rangle = \int \Psi^*(x,t)\, f(x,t)\, \Psi(x,t)\, dx$

Dispersion $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$)

V1 Visa att $\Psi(x,t) = A e^{i(kx-\omega t)}$ är egenfkn. till operatorn $\hat{p} = -i\hbar \frac{d}{dx}$:

$$\hat{p}\Psi = -i\hbar \frac{d}{dx} A e^{i(kx-\omega t)} = -i\hbar (ik) A e^{i(kx-\omega t)} = \underset{\text{egenv.}}{\hbar k}\, \Psi(x,t)$$

OK!

Alltså: Egenvärdet till operatorn $\hat{p} = \hbar k = p$ (rörelsemängd)

$$\langle p\rangle = \int_{-\infty}^{\infty} dx\, \Psi^* \underbrace{\hat{p}\Psi}_{=\hbar k \Psi} = \hbar k \underbrace{\int_{-\infty}^{\infty} |\Psi|^2 dx}_{=1} = \hbar k$$

$$\langle p^2\rangle = \int_{-\infty}^{\infty} dx\, \Psi^* \hat{p}\underbrace{\hat{p}\Psi}_{\hbar k \Psi} = \hbar k \underbrace{\int_{-\infty}^{\infty} \Psi^* \hat{p}\Psi\, dx}_{=\hbar k} = \hbar^2 k^2$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{(\hbar k)^2 - (\hbar k)^2} = 0$$

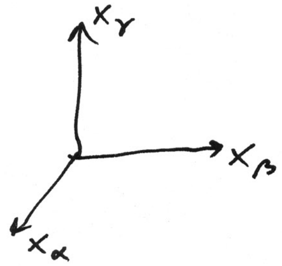
Planvåg med bestämd rörelsemängd, men helt utbredd i rummet.

V9 Oerhört lätt, men bra att göra och komma ihåg

$\Rightarrow$ Gör själv!

V10

a) $[\hat{x}_\alpha, \hat{x}_\beta]$ Operatorer m. egenvärden $x_\alpha, x_\beta \dots$



Dessa kommuterar, dvs $xy = yx$ osv...

Låt kommutatorn verka på en fkn:

$$[\hat{x}_\alpha, \hat{x}_\beta]\psi = (x_\alpha x_\beta - x_\beta x_\alpha)\psi = 0$$

b) $$[\hat{p}_\alpha, \hat{p}_\beta]\psi = \left\{\hat{p}_\alpha \to -i\hbar\frac{\partial}{\partial x_\alpha}\right\} = -\hbar^2\left(\frac{\partial}{\partial x_\alpha}\frac{\partial}{\partial x_\beta} - \frac{\partial}{\partial x_\beta}\frac{\partial}{\partial x_\alpha}\right)\psi = 0$$

(derivatorer kommuterar)

c) $$[\hat{x}_\alpha, \hat{p}_\beta]\psi = -i\hbar\left(x_\alpha\frac{\partial}{\partial x_\beta} - \frac{\partial}{\partial x_\beta}x_\alpha\right)\psi =$$

$$= -i\hbar\left[x_\alpha\frac{\partial}{\partial x_\beta}\psi - \frac{\partial}{\partial x_\beta}(x_\alpha\psi)\right] = -i\hbar\left(x_\alpha\frac{\partial\psi}{\partial x_\beta} - \frac{\partial x_\alpha}{\partial x_\beta}\psi - x_\alpha\frac{\partial\psi}{\partial x_\beta}\right)$$

$$= i\hbar\underbrace{\frac{\partial x_\alpha}{\partial x_\beta}}_{\substack{=1 \text{ om } \alpha=\beta \\ 0 \text{ annars}}}\psi = i\hbar\,\delta_{\alpha,\beta}\psi$$

d) $$[\hat{p}_\alpha, F(x)]\psi(x) = -i\hbar\left[\frac{\partial}{\partial x_\alpha}(F\psi) - F\frac{\partial}{\partial x_\alpha}\psi\right] =$$

$$= -i\hbar\left(\frac{\partial F}{\partial x_\alpha}\psi + F\frac{\partial\psi}{\partial x_\alpha} - F\frac{\partial\psi}{\partial x_\alpha}\right) = -i\hbar\frac{\partial F}{\partial x_\alpha}\psi$$