QM i 2D med rotasjonssymm. $V(r)$ [PCH 5.3]

- myk overgang til 3D
- eksperimentelt mulig: Hvis L_z er så liten at $\pi^2\hbar^2/2mL_z^2 \gg k_BT$, er alle partiklene i tilstander med $n_z = 1$, og "z-frihetsgraden" er "frosset ut", dvs systemet er essensielt 2-dimensjonalt

$(x,y) \rightarrow$ polarkoord. (r, φ)

$$x = r\cos\varphi, \quad y = r\sin\varphi, \quad r = \sqrt{x^2+y^2}, \quad \varphi = \arctan(y/x)$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \ldots = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}$$

[F.eks. med kjerneregel: $\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \varphi}{\partial x}\frac{\partial}{\partial \varphi} = \frac{x}{r}\frac{\partial}{\partial r} - \frac{y/x^2}{1+(y/x)^2}\frac{\partial}{\partial \varphi} =$

$= \cos\varphi\frac{\partial}{\partial r} - \frac{\sin\varphi}{r}\frac{\partial}{\partial \varphi}$; $\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial \varphi}{\partial y}\frac{\partial}{\partial \varphi} = \ldots = \sin\varphi\frac{\partial}{\partial r} + \frac{\cos\varphi}{r}\frac{\partial}{\partial \varphi}$

$$\left.\begin{aligned} \Rightarrow \frac{\partial^2}{\partial x^2} &= \left(\cos\varphi\frac{\partial}{\partial r} - \frac{\sin\varphi}{r}\frac{\partial}{\partial \varphi}\right)\left(\cos\varphi\frac{\partial}{\partial r} - \frac{\sin\varphi}{r}\frac{\partial}{\partial \varphi}\right) = \ldots \\ \frac{\partial^2}{\partial y^2} &= \left(\sin\varphi\frac{\partial}{\partial r} + \frac{\cos\varphi}{r}\frac{\partial}{\partial \varphi}\right)^2 = \ldots \end{aligned}\right\} \Rightarrow \nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}$$]

$\Rightarrow$ TUSL for partikkel med masse μ:

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right)\Psi(r,\varphi) + V(r)\Psi(r,\varphi) = E\Psi(r,\varphi)$$

Setter inn $\Psi(r,\varphi) = R(r)\Phi(\varphi)$ og ganger med $-\frac{2\mu}{\hbar^2}\frac{r^2}{\Psi}$:

$$\underbrace{r^2\left\{\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr} + \frac{2\mu}{\hbar^2}\left[E - V(r)\right]R\right\}}_{\text{kun avhengig av } r} = \underbrace{-\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}}_{\text{kun avh. av } \varphi}$$

$\Rightarrow$ Begge sider av likhetstegnet må være lik en konstant, settes lik m^2

$$\Rightarrow \frac{d^2\Phi}{d\varphi^2} + m^2\Phi = 0$$

[Ligningen for $R(r)$ er vanskeligere, og avh. av formen på $V(r)$]

$$\Rightarrow \Phi(\varphi) \sim e^{im\varphi}$$

$$\Phi(\varphi) = \Phi(\varphi + 2\pi) \Rightarrow e^{im\cdot 2\pi} = 1 \Rightarrow \text{heltallig } m$$

$$\Rightarrow \Psi(r,\varphi) = R(r)\,e^{im\varphi} \quad ; \quad m = 0, \pm 1, \pm 2, \dots$$

Dreieimpuls i 2D:

$$\vec{L} = \vec{r} \times \vec{p} = (x\hat{x} + y\hat{y}) \times (p_x\hat{x} + p_y\hat{y})$$

$$= (xp_y - yp_x)\hat{z} = L_z\hat{z} \quad (= \text{klassisk dreieimpuls i 2D})$$

QM: $p_y \to \hat{p}_y = \frac{\hbar}{i}\frac{\partial}{\partial y}$, $\quad p_x \to \hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$

$$L_z \to \hat{L}_z = x\hat{p}_y - y\hat{p}_x = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

Polarkoord:

$$x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} = r\cos\varphi\left(\sin\varphi\frac{\partial}{\partial r} + \frac{\cos\varphi}{r}\frac{\partial}{\partial\varphi}\right)$$
$$- r\sin\varphi\left(\cos\varphi\frac{\partial}{\partial r} - \frac{\sin\varphi}{r}\frac{\partial}{\partial\varphi}\right) = \frac{\partial}{\partial\varphi}$$

$$\Rightarrow \boxed{\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}}$$

Vi ser at $\hat{L}_z\Psi(r,\varphi) = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}R(r)e^{im\varphi} = m\hbar\,\Psi(r,\varphi)$

$\Rightarrow \Psi(r,\varphi) = R(r)e^{im\varphi}$ er <u>egenfunksjoner</u> for $\hat{L}_z$ med <u>egenverdier</u> $m\hbar$

$\Rightarrow$ Partikler i 2D rot. symm. pot. $V(r)$ har <u>kvantisert dreieimpuls</u>:

$$L_z = 0, \pm\hbar, \pm 2\hbar, \dots$$

Dreieimpuls i 3D [PCH 5.4; DJG ; IØ 5.2]

$$\vec{L} = \vec{r} \times \vec{p} \Rightarrow \hat{\vec{L}} = \vec{r} \times \frac{\hbar}{i} \nabla$$

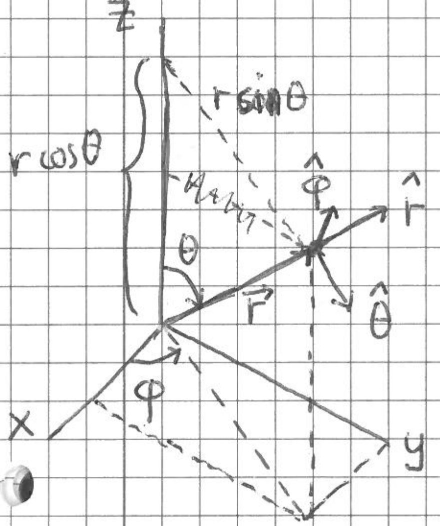
$$\vec{r} = r\,\hat{r}$$

$$\nabla = \hat{r}\,\frac{\partial}{\partial r} + \hat{\theta}\,\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\varphi}\,\frac{1}{r\sin\theta}\frac{\partial}{\partial \varphi}$$

[$df = \nabla f \cdot d\vec{s}$; $d\vec{s} = \hat{r}\,dr + \hat{\theta}\,r\,d\theta + \hat{\varphi}\,r\sin\theta\,d\varphi$

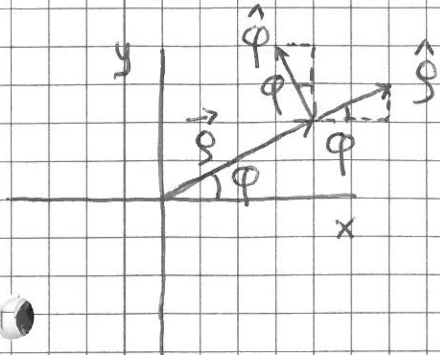
Har dessuten, når $f = f(r,\theta,\varphi)$, at $df = \frac{\partial f}{\partial r}dr + \frac{\partial f}{\partial \theta}d\theta + \frac{\partial f}{\partial \varphi}d\varphi$

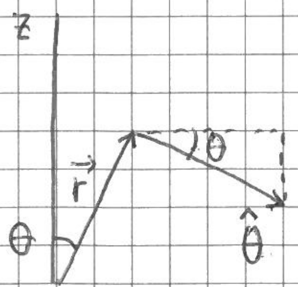
Sammenligning gir $(\nabla f)_r = \frac{\partial f}{\partial r}$, $(\nabla f)_\theta = \frac{1}{r}\frac{\partial f}{\partial \theta}$, $(\nabla f)_\varphi = \frac{1}{r\sin\theta}\frac{\partial f}{\partial \varphi}$]



$$\hat{r} \times \hat{r} = 0$$
$$\hat{r} \times \hat{\theta} = \hat{\varphi}$$
$$\hat{r} \times \hat{\varphi} = -\hat{\theta}$$

$$\Rightarrow \hat{\vec{L}} = \frac{\hbar}{i}\left(\hat{\varphi}\,\frac{\partial}{\partial \theta} - \hat{\theta}\,\frac{1}{\sin\theta}\frac{\partial}{\partial \varphi} \right)$$





$$\hat{\varphi} = -\hat{x}\,\sin\varphi + \hat{y}\,\cos\varphi$$
$$\hat{\rho} = \hat{x}\,\cos\varphi + \hat{y}\,\sin\varphi$$
$$\hat{\theta} = -\hat{z}\,\sin\theta + \hat{\rho}\,\cos\theta$$
$$= -\hat{z}\,\sin\theta$$
$$+ \hat{x}\,\cos\varphi\,\cos\theta$$
$$+ \hat{y}\,\sin\varphi\,\cos\theta$$

$$\Rightarrow \hat{\vec{L}} = \frac{\hbar}{i}\Big\{ -\hat{x}\sin\varphi \frac{\partial}{\partial\theta} + \hat{y}\cos\varphi\frac{\partial}{\partial\theta} + \hat{z}\frac{\partial}{\partial\varphi} - \hat{x}\cos\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi} - \hat{y}\sin\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\Big\}$$

$$\Rightarrow \hat{L}_x = \frac{\hbar}{i}\Big\{-\sin\varphi\frac{\partial}{\partial\theta} - \cos\varphi\cot\theta\frac{\partial}{\partial\varphi}\Big\}$$

$$\hat{L}_y = \frac{\hbar}{i}\Big\{\cos\varphi\frac{\partial}{\partial\theta} - \sin\varphi\cot\theta\frac{\partial}{\partial\varphi}\Big\}$$

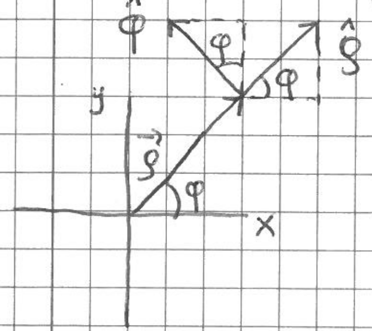
$$\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}$$

Vi trenger også $\hat{\vec{L}}^2 = \hat{\vec{L}}\cdot\hat{\vec{L}}$, som kan regnes ut på (minst) et par måter:

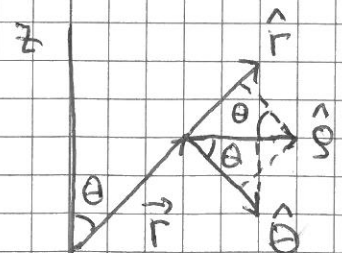
(1) $\hat{\vec{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

(2) $\hat{\vec{L}}^2 = \left(\frac{\hbar}{i}\right)^2\left(\hat{\varphi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}\right)\left(\hat{\varphi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}\right)$

Med (2) trengs $\frac{\partial\hat{\varphi}}{\partial\varphi}$, $\frac{\partial\hat{\varphi}}{\partial\theta}$, $\frac{\partial\hat{\theta}}{\partial\varphi}$ og $\frac{\partial\hat{\theta}}{\partial\theta}$:



$$\hat{\varphi} = -\hat{x}\sin\varphi + \hat{y}\cos\varphi$$
$$\hat{\rho} = \hat{x}\cos\varphi + \hat{y}\sin\varphi$$



$$\hat{z} = \hat{r}\cos\theta - \hat{\theta}\sin\theta$$
$$\hat{\theta} = -\hat{z}\sin\theta + \hat{\rho}\cos\theta$$
$$= -\hat{z}\sin\theta + \hat{x}\cos\varphi\cos\theta + \hat{y}\sin\varphi\cos\theta$$
$$\hat{\rho} = \hat{\theta}\cos\theta + \hat{r}\sin\theta$$

$$\Rightarrow \frac{\partial\hat{\varphi}}{\partial\varphi} = -\hat{x}\cos\varphi - \hat{y}\sin\varphi = -\hat{\rho} = -\hat{\theta}\cos\theta - \hat{r}\sin\theta$$

$$\frac{\partial\hat{\varphi}}{\partial\theta} = 0\ ; \quad \frac{\partial\hat{\theta}}{\partial\varphi} = -\hat{x}\sin\varphi\cos\theta + \hat{y}\cos\varphi\cos\theta = \hat{\varphi}\cos\theta$$

og $\partial\hat{\theta}/\partial\theta = -\hat{z}\cos\theta - \hat{\rho}\sin\theta = -\hat{r}\cos^2\theta + \cancel{\hat{\theta}\sin\theta\cos\theta} - \cancel{\hat{\theta}\sin\theta\cos\theta} - \hat{r}\sin^2\theta = -\hat{r}$

Tror likevel (i) er enklest!

$$\hat{L}_x\hat{L}_x = -\hbar^2\left(-\sin\varphi\frac{\partial}{\partial\theta}-\cos\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right)\left(-\sin\varphi\frac{\partial}{\partial\theta}-\cos\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right)$$

$$= -\hbar^2\Big(\sin^2\varphi\frac{\partial^2}{\partial\theta^2}+\sin\varphi\cos\varphi\left(-\frac{\sin\theta}{\sin\theta}-\frac{\cos^2\theta}{\sin^2\theta}\right)\frac{\partial}{\partial\varphi}+\sin\varphi\cos\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta}\frac{\partial}{\partial\varphi}$$

$$+\cos^2\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta}+\cos\varphi\sin\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\frac{\partial}{\partial\theta}$$

$$-\cos\varphi\sin\varphi\frac{\cos^2\theta}{\sin^2\theta}\frac{\partial}{\partial\varphi}+\cos^2\varphi\frac{\cos^2\theta}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\Big)$$

$$\hat{L}_y\hat{L}_y = -\hbar^2\left(\cos\varphi\frac{\partial}{\partial\theta}-\sin\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right)\left(\cos\varphi\frac{\partial}{\partial\theta}-\sin\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right)$$

$$= -\hbar^2\Big(\cos^2\varphi\frac{\partial^2}{\partial\theta^2}-\cos\varphi\sin\varphi\left(-\frac{\sin\theta}{\sin\theta}-\frac{\cos^2\theta}{\sin^2\theta}\right)\frac{\partial}{\partial\varphi}-\cos\varphi\sin\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta}\frac{\partial}{\partial\varphi}$$

$$+\sin^2\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta}-\sin\varphi\cos\varphi\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\frac{\partial}{\partial\theta}$$

$$+\sin\varphi\cos\varphi\frac{\cos^2\theta}{\sin^2\theta}\frac{\partial}{\partial\varphi}+\sin^2\varphi\frac{\cos^2\theta}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\Big)$$

$$\hat{L}_z\hat{L}_z = -\hbar^2\frac{\partial^2}{\partial\varphi^2}$$

$$\Rightarrow \hat{\vec{L}}^2 = -\hbar^2\left\{\frac{\partial^2}{\partial\theta^2}+\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta}+\frac{\cos^2\theta}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial\varphi^2}\right\}$$

$$= \underline{\underline{-\hbar^2\left\{\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}}}$$

I $\hat{H}$ inngår ∇^2, som i kulekoord. er (uten bevis!)

$$\nabla^2 = \frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\underbrace{\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)}_{=-\hat{\vec{L}}^2/\hbar^2}$$

$\Rightarrow$ Vi kan skrive: (μ = massen)

$$\hat{H} = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{\hat{\vec{L}}^2}{2\mu r^2}+V(r) = \hat{K}_r+\hat{K}_L+V(r)$$

som kan vise seg <u>nyttig</u>! (Vi antar her <u>kulesymm.</u> pot. $V(r)$)

Fra s. 42: $\Delta A \cdot \Delta B \geq \frac{1}{2} \left| \langle i [\hat{A}, \hat{B}] \rangle \right|$

Dvs: Kan ha skarpe verdier for A og B samtidig,

$$\Delta A = \Delta B = 0,$$

(kun) dersom $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0.$

Hvis $\Delta A = \Delta B = 0$, sier vi at A og B er kompatible.

Da må systemet (partikkelen) befinne seg i en tilstand φ som er egentilstand til både $\hat{A}$ og $\hat{B}$:

$$\hat{A}\varphi = A\varphi, \quad \hat{B}\varphi = B\varphi \; ; \qquad \varphi = \text{simultan egenfunksjon til } \hat{A} \text{ og } \hat{B}$$

[Se også PCH 4.1; DJG ; IØ 4.1]

- Kan vi ha skarp energi E og abs.verdi av dreieimpuls, $|\vec{L}|$, samtidig? Dvs: Er $[\hat{H}, \hat{\vec{L}}^2] = 0$?

Ja!

$$[\hat{H}_r, \hat{\vec{L}}^2] = [\underbrace{\hat{K}_r + V(r)}_{\text{kun } r}, \underbrace{\hat{\vec{L}}^2}_{\text{kun } \theta, \varphi}] = 0$$

$$[\hat{K}_L, \hat{\vec{L}}^2] = \frac{1}{2\mu r^2} [\hat{\vec{L}}^2, \hat{\vec{L}}^2] = 0$$

$$\Rightarrow \quad [\hat{H}, \hat{\vec{L}}^2] = 0$$

- Kan vi ha skarp $\vec{L}$? Dvs skarp L_x, L_y og L_z samtidig? Dvs: Er $[\hat{L}_i, \hat{L}_j] = 0$? $(i,j = x,y,z)$

Nei!

$$[\hat{L}_x, \hat{L}_y] = [y\hat{p}_z - z\hat{p}_y \,,\; z\hat{p}_x - x\hat{p}_z]$$
$$= -\hbar^2 \left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \,,\; z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right]$$

Her "overlever" kun $y\frac{\partial}{\partial x}$ og $-x\frac{\partial}{\partial y}$

$$\Rightarrow [\hat{L}_x, \hat{L}_y] = -\hbar^2 \left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} \right) = -\hbar^2 \cdot \left(-\frac{i}{\hbar}\right)\hat{L}_z = i\hbar\hat{L}_z$$

Tilsvarende: $[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$ og $[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$

$\Rightarrow$ Bare <u>en</u> komponent av $\vec{L}$ kan være skarp om gangen!

- Kan vi ha skarp $|\vec{L}|$ og L_i $(i = x,y,z)$ samtidig?

Dvs: Er $[\hat{\vec{L}}^2, \hat{L}_i] = 0$?

Ja! Ser f.eks. på $i = x$.

$$[\hat{L}_x^2, \hat{L}_x] = 0 \quad \text{(selvsagt)}$$
$$[\hat{L}_y^2, \hat{L}_x] = \hat{L}_y\hat{L}_y\hat{L}_x - \hat{L}_x\hat{L}_y\hat{L}_y$$
$$= \hat{L}_y\hat{L}_y\hat{L}_x - \hat{L}_y\hat{L}_x\hat{L}_y + \hat{L}_y\hat{L}_x\hat{L}_y - \hat{L}_x\hat{L}_y\hat{L}_y$$
$$= \hat{L}_y[\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x]\hat{L}_y$$
$$= \hat{L}_y(-i\hbar\hat{L}_z) + (-i\hbar\hat{L}_z)\hat{L}_y$$

$$[\hat{L}_z^2, \hat{L}_x] = \ldots = \hat{L}_z[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z = \hat{L}_z(i\hbar\hat{L}_y) + (i\hbar\hat{L}_y)\hat{L}_z$$
$$= -[\hat{L}_y^2, \hat{L}_x]$$

$$\Rightarrow [\hat{\vec{L}}^2, \hat{L}_x] = 0$$ og tilsvarende blir også

$$[\hat{\vec{L}}^2, \hat{L}_y] = 0, \quad [\hat{\vec{L}}^2, \hat{L}_z] = 0$$

$\Rightarrow$ $L = |\vec{L}|$ og <u>en</u> av komponentene til $\vec{L}$

kan ha skarpe verdier samtidig!

- $\boxed{\text{Dermed, for kulesymm. pot. } V(r)\text{, er } E, |\vec{L}| \text{ og (f.eks.) } L_z \text{ kompatible fysiske størrelser som alle kan være skarpt definert samtidig.}}$

- <u>Hvilke verdier</u> kan L^2 og L_z ha i et kulesymm. pot. $V(r)$?

Svar: $\hbar^2 \ell(\ell+1)$; $\ell = 0, 1, 2, \ldots$ (L^2)

og $m\hbar$; $m = 0, \pm 1, \pm 2, \ldots, \pm \ell$

Dvs: $$\hat{\vec{L}}^2 Y_{\ell m}(\theta, \varphi) = \hbar^2 \ell(\ell+1) Y_{\ell m}(\theta, \varphi)$$

$$\hat{L}_z Y_{\ell m}(\theta, \varphi) = m\hbar Y_{\ell m}(\theta, \varphi)$$ [Se s. 92]

Egenfunksjonene $Y_{\ell m}(\theta, \varphi)$ kalles <u>sfæriske harmoniske</u>.

(Evt. <u>kulefunksjoner.</u>)

Fra s. 92 vet vi at $Y_{\ell m}$ har φ-avhengighet gitt ved $\exp(im\varphi)$. Dvs:

$$Y_{\ell m}(\theta,\varphi) = \Theta(\theta)\cdot\Phi(\varphi) = \Theta(\theta)\, e^{im\varphi}$$

Med $\hat{\vec{L}}^2$ fra s. 95:

$$\hat{\vec{L}}^2 Y_{\ell m}(\theta,\varphi) = -\hbar^2\left\{\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}\Theta(\theta)\, e^{im\varphi}$$

Her er $\frac{\partial^2}{\partial\varphi^2} e^{im\varphi} = -m^2 e^{im\varphi}$.

$$\frac{\partial^2\Theta}{\partial\theta^2} + \frac{\cos\theta}{\sin\theta}\frac{\partial\Theta}{\partial\theta} = \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\cdot\frac{d\Theta}{d\theta}\right)$$

Substituér $x = \cos\theta \Rightarrow dx = -\sin\theta\, d\theta$ og $\sin\theta = \sqrt{1-x^2}$

$$\Rightarrow \frac{d}{\sin\theta\, d\theta}\left(\sin^2\theta\,\frac{d\Theta}{\sin\theta\, d\theta}\right) = \left(-\frac{d}{dx}\right)\left((1-x^2)\cdot\left(-\frac{d\Theta}{dx}\right)\right)$$

$$= \frac{d}{dx}\left[(1-x^2)\frac{d\Theta}{dx}\right]$$

$$= (1-x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx}$$

Egenverdiligningen,

$$\hat{\vec{L}}^2 Y_{\ell m} = \hbar^2 \ell(\ell+1) Y_{\ell m}$$

blir nå

$$-(1-x^2)\Theta'' + 2x\Theta' + \frac{m^2}{1-x^2}\Theta = \ell(\ell+1)\Theta$$

dvs

$$(1-x^2)\Theta'' - 2x\Theta' + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right]\Theta = 0$$

(med <u>heltallig</u> m og foreløpig <u>ukjent</u> ℓ)

Ligningen løses med rekkeutviklingsmetoden, dvs
a la det vi gjorde for harmonisk oscillator.

Detaljene tas ikke her. (Se f.eks. PCH 5.4.5 og 5.4.6)

Vi går heller direkte til løsningene!

$\underline{m=0}$: Legendres diff. ligning,

$$\left[(1-x^2)\frac{d^2}{dx^2} - 2x\frac{d}{dx} + l(l+1)\right] P_l(x) = 0 \; ; \; x = \cos\theta$$

Med normeringsvalget $P_l(1) = 1$ er løsningene <u>Legendre-polynomene</u>

$$P_0(x) = 1 \,, \; P_1(x) = x \,, \; P_2(x) = \frac{1}{2}(3x^2-1) \,, \; \ldots$$

Rodrigues' formel,

$$P_l(x) = \frac{1}{2^l \cdot l!} \frac{d^l}{dx^l} (x^2-1)^l$$

$m=0$ gir $\Phi_m(\varphi) = 1$, slik at

$$Y_{l0} \sim P_l(\cos\theta)$$

dvs

$$Y_{00} \sim 1 \,, \quad Y_{10} \sim \cos\theta \,, \quad Y_{20} \sim 3\cos^2\theta - 1 \,, \ldots$$

(symm.) (antisymm.) (symm.) ...

$m \neq 0$: Må ha $\Theta_\ell^{-m} = \Theta_\ell^{m}$ da m^2 inngår

$\Rightarrow$ nok å ta for seg $m > 0$

Akseptable løsninger er assosierte Legendre-funksjoner,

$$\Theta_\ell^m = P_\ell^m(x) = (1-x^2)^{m/2} \left(\frac{d}{dx}\right)^m P_\ell(x)$$

med $x = \cos\theta$, $(1-x^2)^{m/2} = \sin^m\theta$

$$\Rightarrow \quad Y_{\ell m} \sim P_\ell^m(x)\, e^{im\varphi} \quad ; \quad P_\ell^{-m}(x) = P_\ell^m(x)$$

$$Y_{1\,\pm1} \sim \sin\theta\, e^{\pm i\varphi}$$

$$Y_{2\,\pm1} \sim \sin\theta \cos\theta\, e^{\pm i\varphi}$$

$$Y_{2\,\pm2} \sim \sin^2\theta\, e^{\pm 2i\varphi}$$

osv

Terminologi:

ℓ	0	1	2	3	4	5	
"bokstav"	s	p	d	f	g	h	osv alfabetisk

(sharp) (principal) (diffuse) (fundamental)
fra spektroskopi på 1800-tallet

Kulefunksjonene er <u>ortogonale</u>, så med riktig normering har vi

$$\int Y^*_{\ell m}(\theta,\varphi)\, Y_{\ell' m'}(\theta,\varphi)\, d\Omega = \delta_{\ell\ell'}\,\delta_{mm'}$$

$\sin\theta\, d\theta\, d\varphi$ (romvinkelelement

Danner et såkalt <u>fullstendig sett</u>

$\Rightarrow$ Vilkårlig funksjon $f(\theta,\varphi)$ kan uttrykkes som lineærkombinasjonen

$$f(\theta,\varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} C_{m\ell}\, Y_{\ell m}(\theta,\varphi)$$

<u>Symmetriegenskaper og paritet</u>

[PCH 4.2; DJG ; IØ 4.2]

Paritetsoperator: $\boxed{\hat{P}\,\psi(\vec{r}) = \psi(-\vec{r})}$

dvs $\hat{P}$ "speiler" en funksjon mhp origo. (Evt: <u>Rominversjon</u>)

I 1D: $x \rightarrow -x$

I 2D: $x \rightarrow -x$, $y \rightarrow -y$ evt $r \rightarrow r$, $\varphi \rightarrow \varphi + \pi$

I 3D: $x,y,z \rightarrow -x,-y,-z$ evt $r \rightarrow r$, $\theta \rightarrow \pi - \theta$, $\varphi \rightarrow \varphi + \pi$

Funksjoner uten former for symmetri har generelt ingen bestemt sammenheng mellom $\Psi(\vec{r})$ og $\Psi(-\vec{r})$.

Hvis $\Psi(-\vec{r}) = \Psi(\vec{r})$: $\hat{P}\Psi(\vec{r}) = +1 \cdot \Psi(\vec{r})$ (like paritet)

— " — $\Psi(-\vec{r}) = -\Psi(\vec{r})$: $\hat{P}\Psi(\vec{r}) = -1 \cdot \Psi(\vec{r})$ (odde — " —)

$\Rightarrow$ De to mulige egenverdiene til $\hat{P}$ er $p = \pm 1$.

Egenfunksjoner til $\hat{P}$ er alle funksjoner som oppfyller enten $\Psi(-\vec{r}) = \Psi(\vec{r})$ eller $\Psi(-\vec{r}) = -\Psi(\vec{r})$, dvs funksjoner "med en bestemt paritet".

Sfæriske harmoniske og paritet

$$Y_{\ell m} \sim P_\ell^{|m|}(\cos\theta)\, e^{im\varphi}$$

$$\sim \sin^{|m|}\theta \cdot \{\text{polynom av grad } \ell - |m| \text{ i } \cos\theta\} \cdot e^{im\varphi}$$

Ved rominversjon $(r, \theta, \varphi) \rightarrow (r, \pi - \theta, \varphi + \pi)$:

$$x = \cos\theta \longrightarrow -\cos\theta = -x$$

$$\sin\theta \longrightarrow \sin(\pi - \theta) = \sin\theta$$

$$\Rightarrow \quad P_\ell^{|m|}(\cos\theta) \longrightarrow (-1)^{\ell - |m|} P_\ell^{|m|}(\cos\theta)$$

$$e^{im\varphi} \longrightarrow e^{im\varphi} e^{im\pi} = (-1)^m e^{im\varphi}$$

$$\Rightarrow \boxed{\hat{P}\, Y_{\ell m} = (-1)^\ell\, Y_{\ell m}}$$