Løsning til øving 13 for FY1004, høsten 2007

De sfærisk harmoniske funksjonene $Y_{\ell m}$

En partikkel i tre dimensjoner har posisjon $\vec{r}$ og impuls $\vec{p}$. Dreieimpulsoperatoren $\vec{L} = \vec{r} \times \vec{p}$ er en vektor med komponenter

$$\begin{aligned} L_x &= y p_z - z p_y = -\mathrm{i}\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) , \\ L_y &= z p_x - x p_z = -\mathrm{i}\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) , \\ L_z &= x p_y - y p_x = -\mathrm{i}\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) . \end{aligned}$$

I polarkoordinater r, θ, φ med

$$x = r \sin\theta \cos\varphi \ , \qquad y = r \sin\theta \sin\varphi \ , \qquad z = r \cos\theta \ ,$$

og med de ortogonale enhetsvektorene

$$\begin{aligned} \vec{e}_r &= \frac{\vec{r}}{r} = \sin\theta \, (\cos\varphi \, \vec{e}_x + \sin\varphi \, \vec{e}_y) + \cos\theta \, \vec{e}_z \ , \\ \vec{e}_\theta &= \frac{\partial \vec{e}_r}{\partial \theta} = \cos\theta \, (\cos\varphi \, \vec{e}_x + \sin\varphi \, \vec{e}_y) - \sin\theta \, \vec{e}_z \ , \\ \vec{e}_\varphi &= \frac{1}{\sin\theta} \frac{\partial \vec{e}_r}{\partial \varphi} = - \sin\varphi \, \vec{e}_x + \cos\varphi \, \vec{e}_y \ , \end{aligned}$$

har vi at

$$\nabla = \vec{e}_x \frac{\partial}{\partial x} + \vec{e}_y \frac{\partial}{\partial y} + \vec{e}_z \frac{\partial}{\partial z} = \vec{e}_r \frac{\partial}{\partial r} + \vec{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \vec{e}_\varphi \frac{1}{r \sin\theta} \frac{\partial}{\partial \varphi}$$

og

$$\vec{L} = -\mathrm{i}\hbar \, \vec{r} \times \nabla = -\mathrm{i}\hbar \left(\vec{e}_\varphi \frac{\partial}{\partial \theta} - \vec{e}_\theta \frac{1}{\sin\theta} \frac{\partial}{\partial \varphi} \right) .$$

Det gir at

$$\begin{aligned} L_x &= \vec{e}_x \cdot \vec{L} = -\mathrm{i}\hbar \left(- \sin\varphi \frac{\partial}{\partial \theta} - \cot\theta \cos\varphi \frac{\partial}{\partial \varphi} \right) , \\ L_y &= \vec{e}_y \cdot \vec{L} = -\mathrm{i}\hbar \left(\cos\varphi \frac{\partial}{\partial \theta} - \cot\theta \sin\varphi \frac{\partial}{\partial \varphi} \right) , \\ L_z &= \vec{e}_z \cdot \vec{L} = -\mathrm{i}\hbar \frac{\partial}{\partial \varphi} \ . \end{aligned}$$

Istedenfor operatorene L_x og L_y kan vi bruke operatorene

$$\begin{aligned} L_+ &= L_x + \mathrm{i} L_y = \hbar \, \mathrm{e}^{\mathrm{i}\varphi} \left(\frac{\partial}{\partial \theta} + \mathrm{i} \cot\theta \frac{\partial}{\partial \varphi} \right) , \\ L_- &= L_x - \mathrm{i} L_y = \hbar \, \mathrm{e}^{-\mathrm{i}\varphi} \left(- \frac{\partial}{\partial \theta} + \mathrm{i} \cot\theta \frac{\partial}{\partial \varphi} \right) . \end{aligned}$$

Siden L_x og L_y er Hermiteske, $L_x^\dagger = L_x$ og $L_y^\dagger = L_y$, er $L_- = L_+^\dagger$.

Komponentene av dreieimpulsen oppfyller kommutasjonsrelasjonene

$$[L_x, L_y] = \mathrm{i}\hbar L_z \ , \qquad [L_y, L_z] = \mathrm{i}\hbar L_x \ , \qquad [L_z, L_x] = \mathrm{i}\hbar L_y \ .$$

Eller ekvivalent,

$$[L_z, L_+] = \hbar L_+ \ , \qquad [L_z, L_-] = -\hbar L_- \ , \qquad [L_+, L_-] = 2\hbar L_z \ .$$

Fordi operatorene L_z og $\vec{L}^{\,2} = L_x^2 + L_y^2 + L_z^2$ kommuterer, har de felles egenfunksjoner. Denne oppgaven går ut på å finne de felles egenfunksjonene for L_z og $\vec{L}^{\,2}$, som vi kaller $Y_{\ell m}(\theta, \varphi)$. De er funksjoner av vinklene θ og φ, siden L_z og $\vec{L}^{\,2}$ er vinkeloperatorer som ikke involverer radialkoordinaten r.

a) Bruk uttrykkene for L_x, L_y og L_z gitt ovenfor til å vise at

$$\begin{aligned}\vec{L}^{\,2} = L_x^2 + L_y^2 + L_z^2 &= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\,\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\,\frac{\partial^2}{\partial\varphi^2}\right)\\ &= -\hbar^2\left(\frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\,\sin\theta\,\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\,\frac{\partial^2}{\partial\varphi^2}\right).\end{aligned}$$

Hint: Metoden for å finne et uttrykk for L_x^2, for eksempel, er å operere på en vilkårlig bølgefunksjon $\psi(r,\theta,\varphi)$. Da er $L_x^2\psi = L_x(L_x\psi)$.

Bevis:

$$\begin{aligned}L_x^2\psi &= L_x(L_x\psi) = -\hbar^2\left(-\sin\varphi\,\frac{\partial}{\partial\theta} - \cot\theta\cos\varphi\,\frac{\partial}{\partial\varphi}\right)\left(-\sin\varphi\,\frac{\partial\psi}{\partial\theta} - \cot\theta\cos\varphi\,\frac{\partial\psi}{\partial\varphi}\right)\\ &= -\hbar^2\left(\sin^2\!\varphi\,\frac{\partial^2\psi}{\partial\theta^2} - \frac{\sin\varphi\cos\varphi}{\sin^2\!\theta}\,\frac{\partial\psi}{\partial\varphi} + \cot\theta\sin\varphi\cos\varphi\,\frac{\partial^2\psi}{\partial\theta\,\partial\varphi}\right.\\ &\qquad + \cot\theta\cos^2\!\varphi\,\frac{\partial\psi}{\partial\theta} + \cot\theta\cos\varphi\sin\varphi\,\frac{\partial\psi}{\partial\varphi\,\partial\theta}\\ &\qquad \left. - \cot^2\!\theta\cos\varphi\sin\varphi\,\frac{\partial\psi}{\partial\varphi} + \cot^2\!\theta\cos^2\!\varphi\,\frac{\partial^2\psi}{\partial\varphi^2}\right),\end{aligned}$$

$$\begin{aligned}L_y^2\psi &= L_y(L_y\psi) = -\hbar^2\left(\cos\varphi\,\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\,\frac{\partial}{\partial\varphi}\right)\left(\cos\varphi\,\frac{\partial\psi}{\partial\theta} - \cot\theta\sin\varphi\,\frac{\partial\psi}{\partial\varphi}\right)\\ &= -\hbar^2\left(\cos^2\!\varphi\,\frac{\partial^2\psi}{\partial\theta^2} + \frac{\cos\varphi\sin\varphi}{\sin^2\!\theta}\,\frac{\partial\psi}{\partial\varphi} - \cot\theta\cos\varphi\sin\varphi\,\frac{\partial^2\psi}{\partial\theta\,\partial\varphi}\right.\\ &\qquad + \cot\theta\sin^2\!\varphi\,\frac{\partial\psi}{\partial\theta} - \cot\theta\sin\varphi\cos\varphi\,\frac{\partial\psi}{\partial\varphi\,\partial\theta}\\ &\qquad \left. + \cot^2\!\theta\sin\varphi\cos\varphi\,\frac{\partial\psi}{\partial\varphi} + \cot^2\!\theta\sin^2\!\varphi\,\frac{\partial^2\psi}{\partial\varphi^2}\right),\end{aligned}$$

$$L_z^2\psi = L_z(L_z\psi) = -\hbar^2\,\frac{\partial^2\psi}{\partial\varphi^2}\,,$$

Disse tre resultatene tilsammen gir det resultatet som skulle bevises:

$$\begin{aligned}\vec{L}^{\,2}\psi = (L_x^2 + L_y^2 + L_z^2)\psi &= -\hbar^2\left(\frac{\partial^2\psi}{\partial\theta^2} + \cot\theta\,\frac{\partial\psi}{\partial\theta} + \frac{1}{\sin^2\theta}\,\frac{\partial^2\psi}{\partial\varphi^2}\right)\\ &= -\hbar^2\left(\frac{1}{\sin\theta}\,\frac{\partial}{\partial\theta}\,\sin\theta\,\frac{\partial\psi}{\partial\theta} + \frac{1}{\sin^2\theta}\,\frac{\partial^2\psi}{\partial\varphi^2}\right).\end{aligned}$$

En litt annen måte å regne på gir samme svar litt raskere og enklere. Vi har at

$$\vec{L}^{\,2}\psi = \vec{L}\cdot(\vec{L}\psi) = -\hbar^2\left(\vec{e}_\varphi\,\frac{\partial}{\partial\theta} - \vec{e}_\theta\,\frac{1}{\sin\theta}\,\frac{\partial}{\partial\varphi}\right)\cdot\left(\vec{e}_\varphi\,\frac{\partial\psi}{\partial\theta} - \vec{e}_\theta\,\frac{1}{\sin\theta}\,\frac{\partial\psi}{\partial\varphi}\right).$$

I dette skalarproduktet forenkles mye. Vi har at

$$\vec{e}_\theta\cdot\vec{e}_\theta = \vec{e}_\varphi\cdot\vec{e}_\varphi = 1\,,\qquad \vec{e}_\theta\cdot\vec{e}_\varphi = \vec{e}_\varphi\cdot\vec{e}_\theta = 0\,.$$

Videre er

$$\begin{aligned}
\frac{\partial \vec{e}_\varphi}{\partial \theta} &= 0 \;, \\
\vec{e}_\varphi \cdot \frac{\partial \vec{e}_\theta}{\partial \theta} &= -\vec{e}_\varphi \cdot \vec{e}_r = 0 \;, \\
\vec{e}_\theta \cdot \frac{\partial \vec{e}_\varphi}{\partial \varphi} &= \vec{e}_\theta \cdot (-\cos\varphi\, \vec{e}_x - \sin\varphi\, \vec{e}_y) = -\cos\theta \;, \\
\vec{e}_\theta \cdot \frac{\partial \vec{e}_\theta}{\partial \varphi} &= \vec{e}_\theta \cdot (\cos\theta\, \vec{e}_\varphi) = 0 \;.
\end{aligned}$$

Alt i alt gir det samme formel som tidligere for $\vec{L}^{\,2}\psi$.

b) La ℓ være et ikke-negativt heltall, $\ell = 0, 1, 2, \ldots$, og definer

$$Y_{\ell\ell}(\theta, \varphi) = C_\ell \, \sin^\ell\theta \, \mathrm{e}^{\mathrm{i}\ell\varphi} \;,$$

der C_ℓ er en normeringsfaktor som må bestemmes.

Vis at $L_z\, Y_{\ell\ell} = \ell\hbar\, Y_{\ell\ell}$, at $\vec{L}^{\,2}\, Y_{\ell\ell} = \ell(\ell+1)\hbar^2\, Y_{\ell\ell}$, og at $L_+ Y_{\ell\ell} = 0$.

Bevis:

$$L_z\, Y_{\ell\ell} = -\mathrm{i}\hbar \frac{\partial}{\partial\varphi} \left(C_\ell \, \sin^\ell\theta \, \mathrm{e}^{\mathrm{i}\ell\varphi} \right) = \ell\hbar\, Y_{\ell\ell} \;.$$

Videre er

$$\begin{aligned}
\vec{L}^{\,2}\, Y_{\ell\ell} &= -\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right) \left(C_\ell \, \sin^\ell\theta \, \mathrm{e}^{\mathrm{i}\ell\varphi} \right) \\
&= -\hbar^2\, C_\ell \left(\frac{\ell}{\sin\theta} \frac{\partial}{\partial\theta} (\sin^\ell\theta \cos\theta) - \ell^2 \sin^{\ell-2}\theta \right) \mathrm{e}^{\mathrm{i}\ell\varphi} \\
&= -\hbar^2\, C_\ell \left(\ell^2 \sin^{\ell-2}\theta \cos^2\theta - \ell \sin^\ell\theta - \ell^2 \sin^{\ell-2}\theta \right) \mathrm{e}^{\mathrm{i}\ell\varphi} \\
&= -\hbar^2\, C_\ell \left(-\ell^2 \sin^\ell\theta - \ell \sin^\ell\theta \right) \mathrm{e}^{\mathrm{i}\ell\varphi} = \ell(\ell+1)\hbar^2\, Y_{\ell\ell} \;.
\end{aligned}$$

Og

$$L_+\, Y_{\ell\ell} = \hbar\, \mathrm{e}^{\mathrm{i}\varphi} \left(\frac{\partial}{\partial\theta} + \mathrm{i}\cot\theta \frac{\partial}{\partial\varphi} \right) \left(C_\ell \, \sin^\ell\theta \, \mathrm{e}^{\mathrm{i}\ell\varphi} \right) = 0 \;.$$

I tre dimensjoner normerer vi en bølgefunksjon $\psi = \psi(x, y, z) = \psi(r, \theta, \varphi)$ slik at

$$\int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}y \int_{-\infty}^{\infty} \mathrm{d}z \; |\psi|^2 = \int_{-\infty}^{\infty} \mathrm{d}r \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi \; r^2 \sin\theta \; |\psi|^2 = 1 \;.$$

Vinkelfunksjonene $Y_{\ell m}$ normerer vi slik at

$$\int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi \; \sin\theta \; |Y_{\ell m}(\theta, \varphi)|^2 = 1 \;.$$

Normeringskravet for $Y_{\ell\ell}$ er da at

$$\int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi \; \sin\theta \; |Y_{\ell\ell}|^2 = |C_\ell|^2 \, 2\pi \int_0^\pi \mathrm{d}\theta \; \sin^{2\ell+1}\theta = 1 \;.$$

Vi må beregne integralet

$$I_\ell = \int_0^\pi d\theta \ \sin^{2\ell+1}\theta \ .$$

For $\ell = 0$ har vi at $I_0 = 2$. Ved delvis integrasjon viser vi at for $\ell = 1, 2, 3, \ldots$ er

$$\begin{aligned} I_\ell &= \int_0^\pi d\theta \ \sin^{2\ell+1}\theta = \int_0^\pi d\theta \ \sin\theta \ \sin^{2\ell}\theta = -\cos\theta \ \sin^{2\ell}\theta\Big|_0^\pi + 2\ell \int_0^\pi d\theta \ \cos^2\theta \ \sin^{2\ell-1}\theta \\ &= 2\ell \int_0^\pi d\theta \ (1 - \sin^2\theta) \ \sin^{2\ell-1}\theta = 2\ell(I_{\ell-1} - I_\ell) \ . \end{aligned}$$

Det gir iterasjonsformelen

$$I_\ell = \frac{2\ell}{2\ell+1} \, I_{\ell-1} \ ,$$

med løsning

$$I_\ell = \frac{2 \cdot 4 \cdot \ldots \cdot (2\ell)}{3 \cdot 5 \cdot \ldots \cdot (2\ell+1)} \cdot 2 = \frac{2^{2\ell+1}(\ell!)^2}{(2\ell+1)!} \ .$$

Normeringskonstanten C_ℓ kan inneholde en vilkårlig valgt fasefaktor (et kompleks tall med absoluttverdi 1). Den vanligste konvensjonen (som kanskje ser litt kunstig ut?) er å velge

$$C_\ell = (-1)^\ell \, \frac{\sqrt{(2\ell+1)!}}{2^{\ell+1} \, \ell! \, \sqrt{\pi}} \ .$$

e) De normerte egenfunksjonene $Y_{\ell m} = Y_{\ell m}(\theta, \varphi)$ kan velges slik at

$$\begin{aligned} L_+ Y_{\ell m} &= \hbar \sqrt{\left(\ell + \frac{1}{2}\right)^2 - \left(m + \frac{1}{2}\right)^2} \, Y_{\ell, m+1} \ , \\ L_- Y_{\ell m} &= \hbar \sqrt{\left(\ell + \frac{1}{2}\right)^2 - \left(m - \frac{1}{2}\right)^2} \, Y_{\ell, m-1} \ . \end{aligned}$$

Bruk disse relasjonene (uten bevis) til å finne eksplisitte uttrykk for alle funksjonene $Y_{\ell m}$ for $\ell = 0$, $\ell = 1$ og $\ell = 2$, og $m = \ell, \ell - 1, \ldots, -\ell$.

Det kan vises at $Y_{\ell,-m} = (-1)^m Y_{\ell m}^*$, derfor er det nok å finne $Y_{\ell m}$ for $m \geq 0$.

Vi har umiddelbart at

$$Y_{00} = C_0 = \frac{1}{2\sqrt{\pi}} = \frac{1}{\sqrt{4\pi}} \ .$$

Videre er

$$Y_{11} = C_1 \sin\theta \, e^{i\varphi} = -\frac{\sqrt{6}}{4\sqrt{\pi}} \sin\theta \, e^{i\varphi} = -\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{i\varphi} \ ,$$

$$Y_{10} = \frac{1}{\sqrt{2}\,\hbar} L_- Y_{11} = -\sqrt{\frac{3}{16\pi}} \, e^{-i\varphi} \left(-\frac{\partial}{\partial\theta} + i\cot\theta \, \frac{\partial}{\partial\varphi}\right) \sin\theta \, e^{i\varphi} = \sqrt{\frac{3}{4\pi}} \cos\theta \ .$$

Formelen $Y_{\ell,-m} = (-1)^m Y_{\ell m}^*$ gir at

$$Y_{1,-1} = -Y_{11}^* = \sqrt{\frac{3}{8\pi}} \sin\theta \, e^{-i\varphi} \ .$$

Samme resultat får vi ved å beregne

$$Y_{1,-1} = \frac{1}{\sqrt{2}\,\hbar} L_- Y_{10} = \sqrt{\frac{3}{8\pi}} \, e^{-i\varphi} \left(-\frac{\partial}{\partial\theta} + i\cot\theta \, \frac{\partial}{\partial\varphi}\right) \cos\theta = \sqrt{\frac{3}{8\pi}} \sin\theta \, e^{-i\varphi} \ .$$

Det var alle tre Y_{1m}. Så kommer

$$Y_{22} = C_2 \sin^2\theta \, \mathrm{e}^{2\mathrm{i}\varphi} = \frac{\sqrt{5!}}{8 \cdot 2! \sqrt{\pi}} \sin^2\theta \, \mathrm{e}^{2\mathrm{i}\varphi} = \sqrt{\frac{120}{256\pi}} \sin^2\theta \, \mathrm{e}^{2\mathrm{i}\varphi} = \sqrt{\frac{15}{32\pi}} \sin^2\theta \, \mathrm{e}^{2\mathrm{i}\varphi} \; ,$$

$$\begin{aligned} Y_{21} \;&=\; \frac{1}{2\hbar} L_- Y_{22} = \sqrt{\frac{15}{128\pi}} \, \mathrm{e}^{-\mathrm{i}\varphi} \left(-\frac{\partial}{\partial\theta} + \mathrm{i} \cot\theta \, \frac{\partial}{\partial\varphi} \right) \sin^2\theta \, \mathrm{e}^{2\mathrm{i}\varphi} \\ &=\; -\sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta \, \mathrm{e}^{\mathrm{i}\varphi} \; , \end{aligned}$$

$$\begin{aligned} Y_{20} \;&=\; \frac{1}{\sqrt{6}\,\hbar} L_- Y_{21} = -\sqrt{\frac{5}{16\pi}} \, \mathrm{e}^{-\mathrm{i}\varphi} \left(-\frac{\partial}{\partial\theta} + \mathrm{i} \cot\theta \, \frac{\partial}{\partial\varphi} \right) \sin\theta\cos\theta \, \mathrm{e}^{\mathrm{i}\varphi} \\ &=\; -\sqrt{\frac{5}{16\pi}} \left(-2\cos^2\theta + \sin^2\theta \right) = \sqrt{\frac{5}{16\pi}} \left(3\cos^2\theta - 1 \right) \; , \end{aligned}$$

$$Y_{2,-1} = -Y_{21}^* = \sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta \, \mathrm{e}^{-\mathrm{i}\varphi} \; ,$$

$$Y_{2,-2} = Y_{22}^* = \sqrt{\frac{15}{32\pi}} \sin^2\theta \, \mathrm{e}^{-2\mathrm{i}\varphi} \; .$$

Legg merke til at fortegnet er $+$ for alle $Y_{\ell m}$ med $m \leq 0$, og følgelig $-$ for alle $Y_{\ell m}$ med $m > 0$ og m odde.