Theoretische Physik für LAK III: Übung 9

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Aufgabe 1

Es ist explizit über Auswertung der Ableitungen die Wirkung der Operatoren auf die gegebenen Kugelflächenfunktionen zu berechnen.

$$\begin{aligned}
\hat{L}_z Y_{10} &= -i\hbar \frac{\partial}{\partial\phi}\left(\sqrt{\frac{3}{4\pi}}\cos\theta\right) = -i\hbar * 0 = 0 \\
\hat{L}_z Y_{11} &= -i\hbar \frac{\partial}{\partial\phi}\left(-\sqrt{\frac{3}{8\pi}}\sin\theta\exp[i\phi]\right) \\
&= i\hbar\sqrt{\frac{3}{8\pi}}\sin\theta\frac{\partial}{\partial\phi}\exp[i\phi] \\
&= i\hbar\sqrt{\frac{3}{8\pi}}\sin\theta * i\exp[i\phi] \\
&= -\hbar\sqrt{\frac{3}{8\pi}}\sin\theta\exp[i\phi]
\end{aligned}$$

$$\begin{aligned}
\hat{L}^2 Y_{10} &= -\hbar^2\left(\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right) * \left(\sqrt{\frac{3}{4\pi}}\cos\theta\right) \\
&= -\hbar^2\left(\underbrace{\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\left(\sqrt{\frac{3}{4\pi}}\cos\theta\right)}_{=0} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) * \left(\sqrt{\frac{3}{4\pi}}\cos\theta\right)\right) \\
&= -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\sqrt{\frac{3}{4\pi}}(-\sin\theta)\right) \\
&= \hbar^2\sqrt{\frac{3}{4\pi}}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin^2\theta \\
&= \hbar^2\sqrt{\frac{3}{4\pi}}\frac{1}{\sin\theta} * 2\sin\theta\cos\theta \\
&= 2\hbar^2\sqrt{\frac{3}{4\pi}}\cos\theta
\end{aligned}$$

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\begin{aligned}
\hat{L}^2 Y_{11} &= -\hbar^2 \left(\frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) \right) * \left(-\sqrt{\frac{3}{8\pi}} \sin\theta \exp[i\phi] \right) \\
&= -\hbar^2 \left(\frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \left(-\sqrt{\frac{3}{8\pi}} \sin\theta \exp[i\phi] \right) + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) \left(-\sqrt{\frac{3}{8\pi}} \sin\theta \exp[i\phi] \right) \right) \\
&= -\hbar^2 \left(\frac{1}{\sin^2\theta} \left(-\sqrt{\frac{3}{8\pi}} \sin\theta \right) * i^2 \exp[i\phi] + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \left(-\sqrt{\frac{3}{8\pi}} \exp[i\phi] \right) \cos\theta \right) \\
&= -\hbar^2 \left(\frac{1}{\sin\theta} \sqrt{\frac{3}{8\pi}} \exp[i\phi] - \frac{1}{\sin\theta} \sqrt{\frac{3}{8\pi}} \exp[i\phi] \frac{\partial}{\partial\theta} (\sin\theta\cos\theta) \right) \\
&= -\hbar^2 \frac{1}{\sin\theta} \sqrt{\frac{3}{8\pi}} \exp[i\phi] \left(1 - \frac{\partial}{\partial\theta} (\sin\theta\cos\theta) \right) \\
&= -\hbar^2 \frac{1}{\sin\theta} \sqrt{\frac{3}{8\pi}} \exp[i\phi] \left(1 - \underbrace{(\sin^2\theta - \cos^2\theta)}_{=1-2\sin^2\theta} \right) \\
&= -\hbar^2 \frac{1}{\sin\theta} \sqrt{\frac{3}{8\pi}} \exp[i\phi] \left(1 - (1 - 2\sin^2\theta) \right) \\
&= -\hbar^2 \frac{1}{\sin\theta} \sqrt{\frac{3}{8\pi}} \exp[i\phi] * 2\sin^2\theta \\
&= -2\hbar^2 \sqrt{\frac{3}{8\pi}} \exp[i\phi] \sin\theta
\end{aligned}
$$

$$
\begin{aligned}
\hat{L}_+ Y_{10} &= \hbar \exp[i\phi] \left(\frac{\partial}{\partial\theta} + i\cot\theta \frac{\partial}{\partial\phi} \right) * \left(\sqrt{\frac{3}{4\pi}} \cos\theta \right) \\
&= \hbar \exp[i\phi] \left(\frac{\partial}{\partial\theta} \left(\sqrt{\frac{3}{4\pi}} \cos\theta \right) + i\cot\theta \frac{\partial}{\partial\phi} \left(\sqrt{\frac{3}{4\pi}} \cos\theta \right) \right) \\
&= \hbar \sqrt{\frac{3}{4\pi}} \exp[i\phi] \left(-\sin\theta) + i\cot\theta\cos\theta \underbrace{\frac{\partial}{\partial\phi}(1)}_{=0} \right) \\
&= -\hbar \sqrt{\frac{3}{4\pi}} \exp[i\phi] \sin\theta \\
\hat{L}_+ Y_{11} &= \hbar \exp[i\phi] \left(\frac{\partial}{\partial\theta} + i\cot\theta \frac{\partial}{\partial\phi} \right) * \left(-\sqrt{\frac{3}{8\pi}} \sin\theta \exp[i\phi] \right) \\
&= \hbar \exp[i\phi] \left(\frac{\partial}{\partial\theta} \left(-\sqrt{\frac{3}{8\pi}} \sin\theta \exp[i\phi] \right) + i\cot\theta \frac{\partial}{\partial\phi} \left(-\sqrt{\frac{3}{8\pi}} \sin\theta \exp[i\phi] \right) \right) \\
&= -\hbar \sqrt{\frac{3}{8\pi}} \exp[i\phi] \left(\exp[i\phi] \frac{\partial}{\partial\theta} \sin\theta + i\cot\theta\sin\theta \frac{\partial}{\partial\phi} \exp[i\phi] \right) \\
&= -\hbar \sqrt{\frac{3}{8\pi}} \exp[i\phi] \left(\exp[i\phi] \cos\theta + i\frac{\cos\theta}{\sin\theta} \sin\theta * i\exp[i\phi] \right) \\
&= -\hbar \sqrt{\frac{3}{8\pi}} \exp[i2\phi] (\cos\theta - \cos\theta) = 0
\end{aligned}
$$

$$\begin{aligned}
\hat{L}_- Y_{10} &= \hbar \exp[-i\phi] \left(-\frac{\partial}{\partial\theta} + i \cot\theta \frac{\partial}{\partial\phi} \right) * \left(\sqrt{\frac{3}{4\pi}} \cos\theta \right) \\
&= \hbar \exp[-i\phi] \left(-\frac{\partial}{\partial\theta} \left(\sqrt{\frac{3}{4\pi}} \cos\theta \right) + i \cot\theta \frac{\partial}{\partial\phi} \left(\sqrt{\frac{3}{4\pi}} \cos\theta \right) \right) \\
&= \hbar \sqrt{\frac{3}{4\pi}} \exp[-i\phi] \left(-\frac{\partial}{\partial\theta} \cos\theta + i \cot\theta \frac{\partial}{\partial\phi} \cos\theta \right) \\
&= \hbar \sqrt{\frac{3}{4\pi}} \exp[-i\phi] \left(-(-\sin\theta) + i \cot\theta \cos\theta \underbrace{\frac{\partial}{\partial\phi} 1}_{=0} \right) \\
&= \hbar \sqrt{\frac{3}{4\pi}} \exp[-i\phi] \sin\theta \\
\hat{L}_- Y_{11} &= \hbar \exp[-i\phi] \left(-\frac{\partial}{\partial\theta} + i \cot\theta \frac{\partial}{\partial\phi} \right) * \left(-\sqrt{\frac{3}{8\pi}} \sin\theta \exp[i\phi] \right) \\
&= -\hbar \sqrt{\frac{3}{8\pi}} \exp[-i\phi] \left(-\frac{\partial}{\partial\theta} (\sin\theta \exp[i\phi]) + i \cot\theta \frac{\partial}{\partial\phi} (\sin\theta \exp[i\phi]) \right) \\
&= -\hbar \sqrt{\frac{3}{8\pi}} \exp[-i\phi] \left(-\cos\theta \exp[i\phi]) + i \cot\theta \sin\theta * i \exp[i\phi] \right) \\
&= -\hbar \sqrt{\frac{3}{8\pi}} \underbrace{\exp[-i\phi] \exp[i\phi]}_{=1} (-\cos\theta - \cos\theta) \\
&= 2\hbar \sqrt{\frac{3}{8\pi}} \cos\theta
\end{aligned}$$

Aufgabe 2

a) Der Winkelanteil $\psi(\theta, \phi) = A(1 + \sin\theta \sin\phi)$ einer Wellenfunktion soll durch Kugelflächenfunktionen ausgedrückt werden.

Mit dem Tip vom Aufgabenblatt versuchen wir nun $\psi(\theta, \phi)$ durch Superposition der Kugelflächenfunktionen Y_{00}, Y_{10}, Y_{11} und $Y_{1,-1}$ auszudrücken.

$$\begin{aligned}
&A(1 + \sin\theta \sin\phi = aY_{00} + bY_{10} + cY_{11} + dY_{1,-1} \\
&A(1 + \sin\theta \sin\phi = a\sqrt{\frac{1}{4\pi}} + b\sqrt{\frac{3}{4\pi}} \cos\theta + c \left(-\sqrt{\frac{3}{8\pi}} \sin\theta \exp[i\phi] \right) + d\sqrt{\frac{3}{8\pi}} \sin\theta \exp[-i\phi] \\
&A(1 + \sin\theta \sin\phi = a\sqrt{\frac{1}{4\pi}} + b\sqrt{\frac{3}{4\pi}} \cos\theta + c \left(-\sqrt{\frac{3}{8\pi}} \sin\theta (\cos\phi + i \sin\phi) \right) + d\sqrt{\frac{3}{8\pi}} \sin\theta (\cos\phi - i \sin \\
&A(1 + \sin\theta \sin\phi = a\sqrt{\frac{1}{4\pi}} + b\sqrt{\frac{3}{4\pi}} \cos\theta - c\sqrt{\frac{3}{8\pi}} \sin\theta \cos\phi - c\sqrt{\frac{3}{8\pi}} \sin\theta i \sin\phi \\
&\qquad + d\sqrt{\frac{3}{8\pi}} \sin\theta \cos\phi - d\sqrt{\frac{3}{8\pi}} \sin\theta i \sin\phi
\end{aligned}$$

Wenn man $c = d$ wählt, fallen die Terme mit $\sqrt{\frac{3}{8\pi}} \sin\theta\cos\phi$ raus.

$$A(1+\sin\theta\sin\phi = a\sqrt{\frac{1}{4\pi}} + b\sqrt{\frac{3}{4\pi}}\cos\theta - c\sqrt{\frac{3}{8\pi}}\sin\theta i\sin\phi - c\sqrt{\frac{3}{8\pi}}\sin\theta i\sin\phi$$
$$A(1+\sin\theta\sin\phi = a\sqrt{\frac{1}{4\pi}} + b\sqrt{\frac{3}{4\pi}}\cos\theta - 2c\sqrt{\frac{3}{8\pi}}\sin\theta i\sin\phi$$

Durch Koeffizientenvergleich sieht man sofort, dass $b = 0$. Desweiteren muss gelten

$$A = a\sqrt{\frac{1}{4\pi}} \qquad \Rightarrow a = A/\sqrt{\frac{1}{4\pi}} = A\sqrt{4\pi}$$
$$A\sin\theta\sin\phi = -i2c\sqrt{\frac{3}{8\pi}}\sin\theta\sin\phi$$
$$A = -i2c\sqrt{\frac{3}{8\pi}} \qquad \Rightarrow c = -A/\left(i2\sqrt{\frac{3}{8\pi}}\right) = \frac{-A}{i}\sqrt{\frac{2\pi}{3}}$$

Der Winkelanteil lässt sich also momentan schreiben als

$$\psi(\theta,\phi) = A\sqrt{4\pi}Y_{00} + \frac{-A}{i}\sqrt{\frac{2\pi}{3}}Y_{11} + \frac{-A}{i}\sqrt{\frac{2\pi}{3}}Y_{1,-1}$$

Durch die Normierung auf 1 im gesamten Winkelraum kann dann die Konstante A bestimmt werden.

$$\begin{aligned}
1 &= \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}|\psi(\theta,\phi)|^2\sin\theta d\phi d\theta \\
&= \int_{\theta=0}^{\pi}\sin\theta d\theta\int_{\phi=0}^{2\pi}|(A\sqrt{4\pi}Y_{00} - \frac{A}{i}\sqrt{\frac{2\pi}{3}}Y_{11} - \frac{A}{i}\sqrt{\frac{2\pi}{3}}Y_{1,-1})|^2 d\phi \\
&= \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}(AA^*4\pi Y_{00}Y_{00}^* + AA^*\frac{\sqrt{4\pi}}{i}\sqrt{\frac{2\pi}{3}}Y_{00}Y_{11}^* + AA^*\frac{\sqrt{4\pi}}{i}\sqrt{\frac{2\pi}{3}}Y_{00}Y_{1,-1}^* \\
&- \frac{AA^*}{i}\sqrt{\frac{2\pi}{3}}\sqrt{4\pi}Y_{11}Y_{00} - \frac{AA^*}{i^2}\frac{2\pi}{3}Y_{11}Y_{11}^* - \frac{AA^*}{i^2}\frac{2\pi}{3}Y_{11}Y_{1,-1}^* \\
&- \frac{AA^*}{i}\sqrt{\frac{2\pi}{3}}\sqrt{4\pi}Y_{1,-1}Y_{00} - \frac{AA^*}{i^2}\frac{2\pi}{3}Y_{1,-1}Y_{11}^* - \frac{AA^*}{i^2}\frac{2\pi}{3}Y_{1,-1}Y_{1,-1}^*)\sin\theta d\phi d\theta
\end{aligned}$$

Wir wissen, dass die Yl,m ein Orthonormalsystem bilden. Dann gilt $\int_0^{\pi}\int_0^{2\pi}Y_{l',m'}Y_{l,m}^*\sin\theta d\phi d\theta = \delta(m,m')\delta(l,l')$. Das bedeutet, dass nur die Terme erhalten bleiben, bei denen $m = m'$ und $l = l'$.

$$\begin{aligned}
1 &= \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}AA^*4\pi Y_{00}Y_{00}^*\sin\theta d\phi d\theta + \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} -\frac{AA^*}{i^2}\frac{2\pi}{3}Y_{11}Y_{11}^*\sin\theta d\phi d\theta \\
&+ \int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} -\frac{AA^*}{i^2}\frac{2\pi}{3}Y_{1,-1}Y_{1,-1}^*\sin\theta d\phi d\theta \\
1 &= AA^*4\pi + AA^*\frac{2\pi}{3} + AA^*\frac{2\pi}{3} \\
1 &= AA^*\frac{16\pi}{3} \\
A^2 &= \frac{3}{16\pi} \qquad \Rightarrow A = \pm\sqrt{\frac{3}{16\pi}}
\end{aligned}$$

Somit ergibt sich $a = \pm\sqrt{\frac{1}{8}}i$ und $c = \pm\sqrt{\frac{3}{4}}$.

b)