4.3 Eigenfunktionen von $\vec{L}^2$ und L_3

Wir wissen: $[L_i, r] = 0$, also kann L_i keine Ableitungen nach r enthalten

→ transformiere auf Kugelkoordinaten und drücke L_1, L_2, L_3 durch Ableitungen nach θ, φ aus

$$x = r \sin\theta \cos\varphi \equiv x_1$$
$$y = r \sin\theta \sin\varphi \equiv x_2$$
$$z = r \cos\theta \equiv x_3$$

Dann ist

$$\vec{x} = r \hat{e}_r$$
$$\vec{\nabla} = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\varphi \frac{1}{r \sin\theta} \frac{\partial}{\partial \varphi}$$

$$\vec{L} = \frac{\hbar}{i} \vec{x} \times \vec{\nabla}$$
$$= \frac{\hbar}{i} r \hat{e}_r \times \left\{ \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\varphi \frac{1}{r \sin\theta} \frac{\partial}{\partial \varphi} \right\}$$

$\{\hat{e}_r, \hat{e}_\theta, \hat{e}_\varphi\}$ bilden ein Rechtssystem

$$\hat{e}_r \times \hat{e}_\theta = \hat{e}_\varphi, \quad \hat{e}_\theta \times \hat{e}_\varphi = \hat{e}_r, \quad \hat{e}_\varphi \times \hat{e}_r = \hat{e}_\theta$$

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

$$\frac{\partial}{\partial\varphi} = \frac{\partial x}{\partial\varphi}\frac{\partial}{\partial x} + \frac{\partial y}{\partial\varphi}\frac{\partial}{\partial y} + \frac{\partial z}{\partial\varphi}\frac{\partial}{\partial z}$$

$$\left(\equiv \sum_{i=1}^{3} \frac{\partial x_i}{\partial\varphi}\frac{\partial}{\partial x_i} \right)$$

$$= -y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y} = \frac{i}{\hbar}\overbrace{\left(x_1 p_2 - x_2 p_1\right)}^{L_3} = \frac{i}{\hbar} L_3 = i\, l_3$$

$$\Rightarrow \quad L_3 = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}, \quad l_3 = -i\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial\theta} = \sum_{i=1}^{3} \frac{\partial x_i}{\partial\theta}\frac{\partial}{\partial x_i}$$

$$= \cos\varphi\left(x_3\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_3}\right) - \sin\varphi\left(x_2\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_2}\right)$$

$$+ \underbrace{\cos\varphi\; x_1\frac{\partial}{\partial x_3} + \sin\varphi\; x_2\frac{\partial}{\partial x_3} - r\sin\theta\frac{\partial}{\partial x_3}}_{=0 \text{ after inserting } x_{1,2}(r,\theta,\varphi)}$$

$$= i\left(\cos\varphi\; l_2 - \sin\varphi\; l_1\right) \qquad [1]$$

Außerdem: $\vec{x}\cdot\vec{l} = \vec{x}\cdot(\vec{x}\times\vec{p}) = 0$

$$x_1 l_1 + x_2 l_2 + x_3 l_3 = 0$$

$$\Rightarrow r\sin\theta\cos\varphi\; l_1 + r\sin\theta\sin\varphi\; l_2 = -r\cos\theta\; l_3 \quad \Big|\; \frac{1}{r\cos\theta}$$

$$\tan\theta\left(\cos\varphi\; l_1 + \sin\varphi\; l_2\right) = -l_3 \qquad [2]$$

$$-\sin\varphi\, l_1 + \cos\varphi\, l_2 = -i\frac{\partial}{\partial\theta} \qquad [1]$$

$$\cos\varphi\, l_1 + \sin\varphi\, l_2 = \cot\theta\, i\frac{\partial}{\partial\varphi} \qquad [2]$$

$-\sin\varphi\,[1] + \cos\varphi\,[2]$: $\quad l_1 = i\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)$

$\cos\varphi\,[1] + \sin\varphi\,[2]$: $\quad l_2 = i\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)$

$$l_3 = -i\frac{\partial}{\partial\varphi}$$

Jetzt: Betrachte $\vec{l}^{\,2} = l_+ l_- + l_3^2 - l_3$ und drücke $l_+ l_-$ und $\vec{l}^{\,2}$ durch Ableitungen nach θ, φ aus.

$$l_+ l_- = (l_1 + il_2)(l_1 - il_2)$$

$$l_1 + il_2 = (i\sin\varphi + \cos\varphi)\frac{\partial}{\partial\theta} + (\cos\varphi + i\sin\varphi)\, i\cot\theta\frac{\partial}{\partial\varphi}$$

$$= e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right)$$

$$l_1 - il_2 = e^{-i\varphi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right)$$

$$\Rightarrow l_+ l_- = e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) e^{-i\varphi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right)$$

$$= \ldots = -\frac{\partial^2}{\partial\theta^2} - i\frac{\partial}{\partial\varphi} - \cot\theta\frac{\partial}{\partial\theta} - \cot^2\theta\frac{\partial^2}{\partial\varphi^2}$$

Daher:

$$\vec{l}^{\,2} = l_+ l_- + l_3^2 - l_3 = l_+ l_- - \frac{\partial^2}{\partial\varphi^2} + i\,\frac{\partial}{\partial\varphi}$$

$$= -\frac{\partial^2}{\partial\theta^2} - \underbrace{(1+\cot^2\theta)}_{1/\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} - \cot\theta\,\frac{\partial}{\partial\theta}$$

$$\cot\theta = \frac{\cos\theta}{\sin\theta} = \frac{1}{\sin\theta}\,\frac{\partial \sin\theta}{\partial\theta}$$

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

$$= -\left\{\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\left[\sin\theta\,\frac{\partial}{\partial\theta}\left(\frac{\partial}{\partial\theta}\right) + \left(\frac{\partial\sin\theta}{\partial\theta}\right)\frac{\partial}{\partial\theta}\right]\right\}$$

$$= -\left\{\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right)\right\}$$

Vergleiche: Laplace-Operator in Kugelkoordinaten

$$\Delta = \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left\{\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right)\right\}$$

$$= \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\,\Delta_{\theta,\varphi}$$

Winkelanteil

Vergleich mit $\vec{l}^{\,2}$ ergibt

$$\boxed{\vec{l}^{\,2} = -\Delta_{\theta,\varphi} \quad ; \quad \vec{L}^{\,2} = -\hbar^2\,\Delta_{\theta,\varphi}}$$

Nach diesen länglichen Vorbetrachtungen bestimmen wir nun die ... →

Eigenfunktionen von $\vec{l}^2, l_3$

Ortsdarstellung: $|l, m\rangle \doteq Y_{lm}(\theta, \varphi)$

(denn wegen $[L_i, r] = 0$ können L_i keine Ableitungen nach r enthalten)

Wegen $l_3 |l, m\rangle = -i \frac{\partial}{\partial \varphi} Y_{lm}(\theta,\varphi) = m\, Y_{lm}(\theta,\varphi)$

muss $Y_{lm}(\theta,\varphi)$ proportional zu $e^{im\varphi}$ sein:

$$Y_{lm}(\theta,\varphi) = g_{lm}(\theta)\, e^{im\varphi}$$

$$-i \frac{\partial}{\partial\varphi} Y_{lm}(\theta,\varphi) = g_{lm}(\theta)\,(-i)\, im\, e^{im\varphi} = m\, g_{lm}(\theta)\, e^{im\varphi}$$

$$= m\, Y_{lm}(\theta,\varphi) \quad \checkmark$$

Betrachte nun

$$l_+ |l, l\rangle = 0$$

$$\Leftrightarrow \underbrace{e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i \cot\theta \frac{\partial}{\partial\varphi}\right)}_{l_+} \underbrace{g_{ll}(\theta)\, e^{il\varphi}}_{Y_{ll}(\theta,\varphi)} = 0$$

$\left[\frac{\partial}{\partial\varphi} e^{il\varphi} = il\, e^{il\varphi}\right]$

$$e^{i(l+1)\varphi}\left(\frac{\partial}{\partial\theta} - l\cot\theta\right) g_{ll}(\theta) = 0$$

$$\Rightarrow \frac{d\, g_{ll}(\theta)}{d\theta} = l \cot\theta\; g_{ll}(\theta)$$

$$\Rightarrow \int d(\ln g_{ll}) = l \int \cot\theta \, d\theta + c_l$$

$$\left[\int \cot\theta \, d\theta = \int \frac{\cos\theta}{\sin\theta} d\theta = \int \frac{\sin'\theta}{\sin\theta} d\theta = \int d(\ln \sin\theta) \right.$$

wg. $\int \frac{f'}{f} dx = \ln f + c$ $\left.\right]$

$$\Rightarrow \int d(\ln g_{ll}) = l \int d(\ln \sin\theta) + c_l$$

$$\Rightarrow g_{ll}(\theta) = (\sin\theta)^l \cdot c_l$$

Also ist die Eigenfunktion für $m = m_{max} = l$:

$$Y_{ll}(\theta, \varphi) = c_l \, (\sin\theta)^l \, e^{il\varphi}$$

Bestimme c_l aus Normierungsbedingung:

$$\int d\Omega \, |Y_{ll}|^2 = |c_l|^2 \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \, \sin\theta \, (\sin\theta)^{2l} \overset{!}{=} 1$$

$$\Rightarrow |c_l|^2 \, 2\pi \int_0^{\pi} d\theta \, (\sin\theta)^{2l+1} = 1$$

$$\Rightarrow |c_l|^2 = \frac{1}{4\pi} \frac{2l+1}{4^l} \binom{2l}{l}$$

Eigenfunktionen $Y_{lm}(\theta,\varphi)$ für $m < l$ erhält man durch sukzessive Anwendung des **Leiteroperators l_-:**

$$l_- \, g_{ll}(\theta)\, e^{il\varphi} = e^{-i\varphi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\varphi}\right) g_{ll}(\theta)\, e^{il\varphi}$$

$$= -\left(\frac{\partial}{\partial\theta} + l\cot\theta\right) g_{ll}(\theta)\, e^{i(l-1)\varphi}$$

$$= -(\sin\theta)^{-l}\frac{\partial}{\partial\theta}(\sin\theta)^l\, g_{ll}(\theta)\, e^{i(l-1)\varphi}$$

$$= \underbrace{(\sin\theta)^{-(l-1)}\frac{d}{d\cos\theta}(\sin\theta)^l\, g_{ll}(\theta)}_{g_{l,l-1}(\theta)}\; e^{\overset{\uparrow\; m=l-1\;\checkmark}{i(l-1)\varphi}}$$

$$\boxed{\begin{aligned}&\frac{\partial}{\partial\theta}(\sin\theta)^l = l(\sin\theta)^{l-1}\cos\theta\\ &= l(\sin\theta)^l\cot\theta\\ &(\sin\theta)^{-l}\frac{\partial}{\partial\theta}(\sin\theta)^l = l\cot\theta\end{aligned}}$$

$$\boxed{\begin{aligned}&\frac{d}{d(\cos\theta)} = \frac{1}{-\sin\theta}\frac{d}{d\theta}\\ &\Rightarrow \frac{d}{d\theta} = -\sin\theta\frac{d}{d\cos\theta}\end{aligned}}$$

Nochmalige Anwendung von l_-:

$$l_- \, g_{l,l-1}(\theta)\, e^{i(l-1)\varphi}$$

$$= (\sin\theta)^{-(l-2)}\frac{d}{d\cos\theta}(\sin\theta)^{l-1}\, g_{l,l-1}(\theta)\, e^{i(l-2)\varphi}$$

$$= (\sin\theta)^{-(l-2)}\frac{d}{d\cos\theta}\underbrace{(\sin\theta)^{l-1}\,(\sin\theta)^{-(l-1)}}_{1}\frac{d}{d\cos\theta}(\sin\theta)^l\, g_{ll}(\theta)\, e^{i(l-2)\varphi}$$

$$= (\sin\theta)^{-(l-2)}\left(\frac{d}{d\cos\theta}\right)^2(\sin\theta)^l\, g_{ll}(\theta)\, e^{i(l-2)\varphi}$$

Nach $(l-m)$-maliger Anwendung: (wie beim harm. Osz.)

$$(L_-)^{l-m} \, g_{ll}(\theta)\, e^{il\varphi}$$

$$= (\sin\theta)^{-(l-l+m)} \left(\frac{d}{d\cos\theta}\right)^{l-m} (\sin\theta)^l \, g_{ll}(\theta)\, e^{i(l-l+m)\varphi}$$

$$= (\sin\theta)^{-m} \left(\frac{d}{d\cos\theta}\right)^{l-m} (\sin\theta)^l \underbrace{g_{ll}(\theta)}_{c_l (\sin\theta)^l} e^{im\varphi}$$

$$= c_l \, (\sin\theta)^{-m} \left(\frac{d}{d\cos\theta}\right)^{l-m} (\sin\theta)^{2l} \, e^{im\varphi} \propto Y_{lm}(\theta,\varphi)$$

Mit der korrekten Normierung findet man

$$Y_{lm}(\theta,\varphi) = \frac{(-)^l}{2^l \, l!} \left(\frac{2l+1}{4\pi}\,\frac{(l+m)!}{(l-m)!}\right)^{1/2} (\sin\theta)^{-m} \times \frac{d^{l-m}}{d(\cos\theta)^{l-m}} (\sin\theta)^{2l} \, e^{im\varphi}$$

$Y_{lm}(\theta,\varphi)$ heißen Kugelflächenfunktionen

(Kugelfunktionen, "spherical harmonics")

4.3 Eigenfunktionen von $\vec{L}^2$ und L_3

Gradient in krummlinigen Koordinaten:

$$\vec{x} = x\,\hat{e}_x + y\,\hat{e}_y + z\,\hat{e}_z \equiv x_1\,\hat{e}_1 + x_2\,\hat{e}_2 + x_3\,\hat{e}_3 = q_1\,\hat{\eta}_1 + q_2\,\hat{\eta}_2 + q_3\,\hat{\eta}_3$$

$\hat{\eta}_i$: Basisvektoren in krummlinigen Koordinaten

Maßstabsfaktoren:

$$h_i := \left|\frac{\partial\vec{x}}{\partial q_i}\right|, \qquad \hat{\eta}_i = \left(\frac{\partial\vec{x}}{\partial q_i}\right)\frac{1}{h_i}$$

Gradient:

$$\vec{\nabla} = \sum_{i=1}^{3}\hat{\eta}_i\,\frac{1}{h_i}\,\frac{\partial}{\partial q_i}$$

Kugelkoordinaten: $x \equiv x_1 = r\sin\theta\cos\varphi, \quad y \equiv x_2 = r\sin\theta\sin\varphi, \quad z \equiv x_3 = r\cos\theta$

$$h_r = \left|\frac{\partial\vec{x}}{\partial r}\right| = 1, \quad h_\theta = \left|\frac{\partial\vec{x}}{\partial\theta}\right| = r, \quad h_\varphi = \left|\frac{\partial\vec{x}}{\partial\varphi}\right| = r\sin\theta$$

$$\vec{x} = x_1\,\hat{e}_1 + x_2\,\hat{e}_2 + x_3\,\hat{e}_3 = r\,\hat{e}_r$$

$$\Rightarrow \quad \vec{\nabla} = \hat{e}_r\,\frac{\partial}{\partial r} + \hat{e}_\theta\,\frac{1}{r}\,\frac{\partial}{\partial\theta} + \hat{e}_\varphi\,\frac{1}{r\sin\theta}\,\frac{\partial}{\partial\varphi}$$

$\{\hat{e}_r, \hat{e}_\theta, \hat{e}_\varphi\}$ bilden ein Rechtssystem:

$$\hat{e}_r \times \hat{e}_\theta = \hat{e}_\varphi\,, \qquad \hat{e}_\theta \times \hat{e}_\varphi = \hat{e}_r\,, \qquad \hat{e}_\varphi \times \hat{e}_r = \hat{e}_\theta$$

Kugelkoordinaten: $x \equiv x_1 = r\sin\theta\cos\varphi, \quad y \equiv x_2 = r\sin\theta\sin\varphi, \quad z \equiv x_3 = r\cos\theta$

$$\frac{\partial}{\partial\varphi} = \sum_{i=1}^{3} \frac{\partial x_i}{\partial\varphi}\frac{\partial}{\partial x_i} \quad \text{mit} \quad \frac{\partial x_1}{\partial\varphi} = -x_2\,, \quad \frac{\partial x_2}{\partial\varphi} = x_1\,, \quad \frac{\partial x_3}{\partial\varphi} = 0\,,$$

$$\frac{\partial}{\partial\theta} = \sum_{i=1}^{3} \frac{\partial x_i}{\partial\theta}\frac{\partial}{\partial x_i} \quad \text{mit} \quad \frac{\partial x_1}{\partial\theta} = x_3\cos\varphi\,, \quad \frac{\partial x_2}{\partial\theta} = x_3\sin\varphi\,, \quad \frac{\partial x_3}{\partial\theta} = r\sin\theta\,,$$

$$\Rightarrow \quad \frac{\partial}{\partial\varphi} = i\,\ell_3\,, \quad \frac{\partial}{\partial\theta} = i\,(\cos\varphi\,\ell_2 - \sin\varphi\,\ell_1) \quad \Rightarrow \quad -\sin\varphi\,\ell_1 + \cos\varphi\,\ell_2 = -i\frac{\partial}{\partial\theta} \qquad [1]$$

$$x_1\ell_1 + x_2\ell_2 + x_3\ell_3 \equiv \vec{x}\cdot\vec{\ell} = \vec{x}\cdot(\vec{x}\times\vec{p}) = 0$$

$$\Rightarrow \quad \tan\theta\,(\cos\varphi\,\ell_1 + \sin\varphi\,\ell_2) = -\ell_3 \qquad \Rightarrow \quad \cos\varphi\,\ell_1 + \sin\varphi\,\ell_2 = i\cot\theta\,\frac{\partial}{\partial\varphi} \qquad [2]$$

$$-\sin\varphi\,\ell_1 + \cos\varphi\,\ell_2 = -i\frac{\partial}{\partial\theta} \qquad [1] \qquad\qquad \cos\varphi\,\ell_1 + \sin\varphi\,\ell_2 = i\cot\theta\,\frac{\partial}{\partial\varphi} \qquad [2]$$

$$-\sin\varphi\,\text{“[1]”} + \cos\varphi\,\text{“[2]”}: \quad \ell_1 = i\left(\ \sin\varphi\,\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\,\frac{\partial}{\partial\varphi}\right)$$

$$\cos\varphi\,\text{“[1]”} + \sin\varphi\,\text{“[2]”}: \quad \ell_2 = i\left(-\cos\varphi\,\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\,\frac{\partial}{\partial\varphi}\right) \qquad \ell_3 = -i\,\frac{\partial}{\partial\varphi}$$

Drücke $\vec{\ell}^{\,2} = \ell_+\,\ell_- + \ell_3^2 - \ell_3\,, \quad \ell_+\,\ell_- = (\ell_1 + i\ell_2)\,(\ell_1 - i\ell_2)$ durch Ableitungen nach θ und φ aus:

$$\ell_1 + i\ell_2 = \mathrm{e}^{i\varphi}\left(\ \frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\varphi}\right), \quad \ell_1 - i\ell_2 = \mathrm{e}^{-i\varphi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\varphi}\right)$$

$$\Rightarrow \quad \ell_+\ell_- = \mathrm{e}^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\varphi}\right)\mathrm{e}^{-i\varphi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\varphi}\right)$$

$$= \ldots = -\frac{\partial^2}{\partial\theta^2} - i\,\frac{\partial}{\partial\varphi} - \cot\theta\,\frac{\partial}{\partial\theta} - \cot^2\theta\,\frac{\partial^2}{\partial\varphi^2} \qquad\qquad \ell_3^3 - \ell^3 = -\frac{\partial^2}{\partial\varphi^2} + i\,\frac{\partial}{\partial\varphi}$$