8. Drehimpuls

Bahndrehimpulsoperator:

$$\hat{\vec{L}} := \hat{\vec{r}} \times \hat{\vec{p}} \quad \text{bzw.} \quad \hat{L}_i := \varepsilon_{ijk}\, \hat{r}_j \hat{p}_k \qquad i,j,k = 1,2,3$$

(Komponentenschreibweise)

Hermitizität:

$$\hat{L}_i^{\dagger} = \varepsilon_{ijk} \left(\hat{r}_j \hat{p}_k \right)^{\dagger}$$

$$= \varepsilon_{ijk}\, \hat{p}_k^{\dagger} \hat{r}_j^{\dagger}$$

$$= \varepsilon_{ijk}\, \hat{p}_k \hat{r}_j$$

$$= \varepsilon_{ijk}\, \hat{r}_j \hat{p}_k$$

$$= \hat{L}_i$$

Kommutatorrelationen:

$$[\hat{L}_j, \hat{L}_k] = \varepsilon_{jnm} \varepsilon_{kil} \left[\hat{r}_n \hat{p}_m , \hat{r}_i \hat{p}_l \right]$$

$$= \varepsilon_{jnm} \varepsilon_{kil} \left(\hat{r}_n \left[\hat{p}_m , \hat{r}_i \hat{p}_l \right] + \left[\hat{r}_n , \hat{r}_i \hat{p}_l \right] \hat{p}_m \right)$$

$$= \varepsilon_{jnm} \varepsilon_{kil} \left(\hat{r}_n (-i\hbar \delta_{mi}) \hat{p}_l + \hat{r}_i (i\hbar \delta_{nl}) \hat{p}_m \right)$$

$$= i\hbar \left(-\varepsilon_{jnm} \varepsilon_{kml}\, \hat{r}_n \hat{p}_l + \varepsilon_{jnm} \varepsilon_{kin}\, \hat{r}_i \hat{p}_m \right)$$

$$= i\hbar \Big(- \underbrace{\varepsilon_{jim} \varepsilon_{kml}}_{\substack{= \varepsilon_{jim} \varepsilon_{lkm} \\ = \delta_{jl}\delta_{ik} - \delta_{jk}\delta_{il}}} + \underbrace{\varepsilon_{jnl} \varepsilon_{kin}}_{\substack{= \varepsilon_{ljn} \varepsilon_{kin} \\ = \delta_{lk}\delta_{ji} - \delta_{li}\delta_{jk}}} \Big) \hat{r}_i \hat{p}_l$$

(Umbenennung der Indizes)

$$= i\hbar \left(-\delta_{je}\delta_{ik} + \delta_{ek}\delta_{ji} \right) \hat{r}_i \hat{p}_e$$

$$= i\hbar\, \varepsilon_{jkn} \underbrace{\varepsilon_{ien} \hat{r}_i \hat{p}_e}_{= \hat{L}_n}$$

Also:

$$\boxed{\left[\hat{L}_j, \hat{L}_k \right] = i\hbar\, \varepsilon_{jkn} \hat{L}_n}$$

Betragsquadrat des Drehimpulsoperators:

$$\hat{\vec{L}}^2 = \hat{L}_i \hat{L}_i = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

mit

$$[\hat{\vec{L}}^2, \hat{L}_i] = [\hat{L}_j \hat{L}_j, \hat{L}_i]$$

$$= \hat{L}_j [\hat{L}_j, \hat{L}_i] + [\hat{L}_j, \hat{L}_i] \hat{L}_j$$

$$= i\hbar \underbrace{\varepsilon_{jin}}_{\substack{\text{anti-}\\ \text{symmetrisch}\\ \text{in } (j,n)}} \underbrace{(\hat{L}_j \hat{L}_n + \hat{L}_n \hat{L}_j)}_{\text{symmetrisch}}$$

$$= 0$$

Also:

$$\boxed{[\hat{\vec{L}}^2, \hat{L}_i] = 0}$$

8.2 Eigenwerte der Drehimpulskomponenten

Ortsdarstellung:

$$\hat{L}_z = \varepsilon_{3jk} \hat{r}_j \hat{p}_k = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \mathrel{\hat{=}} x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right)$$

Kugelkoordinaten:

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

Ableitung:

$$\frac{\partial}{\partial\varphi} = \frac{\partial x}{\partial\varphi}\frac{\partial}{\partial x} + \frac{\partial y}{\partial\varphi}\frac{\partial}{\partial y} + \frac{\partial z}{\partial\varphi}\frac{\partial}{\partial z} \qquad \text{(Kettenregel)}$$

$$= -r\sin\theta\sin\varphi\frac{\partial}{\partial x} + r\sin\theta\cos\varphi\frac{\partial}{\partial y}$$

$$= -y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}$$

Also:

$$\boxed{\hat{L}_z \mathrel{\hat{=}} -i\hbar\frac{\partial}{\partial\varphi}} \quad \text{in Ortsdarstellung}$$

Eigenwertgleichung:

$$\hat{L}_z |m\rangle = \hbar m |m\rangle \quad \text{bzw.} \quad -i\hbar \frac{\partial}{\partial \varphi} \psi_m(r,\theta,\varphi) = \hbar m \, \psi_m(r,\theta,\varphi)$$

(Ortsraum)

Separationsansatz:

$$\psi_m(r,\theta,\varphi) = f(r,\theta)\, g_m(\varphi)$$

Lösung:

$$-i\hbar \frac{\partial}{\partial \varphi} g_m(\varphi) = \hbar m \, g_m(\varphi) \Rightarrow g_m(\varphi) = e^{im\varphi}$$

Stetigkeit der Wellenfunktion:

$$\psi_m(r,\theta,0) \overset{!}{=} \psi_m(r,\theta,2\pi) \Rightarrow g_m(0) = g_m(2\pi)$$

$$\Rightarrow e^{im2\pi} = 1$$

Eigenwerte von $\hat{L}_z$:

$$\boxed{\hbar m \quad \text{mit} \quad m \in \mathbb{Z}}$$

8.3 Drehimpulsalgebra

Algebraische Definition (Drehimpulsoperator):

$$\boxed{\begin{aligned}[\hat{J}_j, \hat{J}_k] &= i\hbar\, \varepsilon_{jkn} \hat{J}_n \\ [\hat{\vec{J}}^2, \hat{J}_i] &= 0\end{aligned}}$$

Gleichzeitige Diagonalisierung von $\hat{\vec{J}}^2$ und $\hat{J}_z$:

$$\boxed{\begin{aligned}\hat{\vec{J}}^2 |j,m\rangle &= \hbar^2 j(j+1) |j,m\rangle \\ \hat{J}_z |j,m\rangle &= \hbar m |j,m\rangle\end{aligned}}$$

Orthonormalsystem:

$$\boxed{\langle j,m | j',m'\rangle = \delta_{jj'} \delta_{mm'}}$$

Bemerkung:

- Eigenwert von $\hat{\vec{J}}^2$ nicht-negativ ($j \geq 0$):

  $\hbar^2 j(j+1) = \langle j,m|\hat{\vec{J}}^2|j,m\rangle = \|\hat{\vec{J}}\,|j,m\rangle\|^2 \geq 0$

Leiteroperator (Drehimpuls):

$$\hat{J}_\pm = \hat{J}_x \pm i \hat{J}_y$$

Kommutatorrelationen:

$$\boxed{\begin{aligned} [\hat{J}_+, \hat{J}_-] &= 2\hbar \hat{J}_z \\ [\hat{J}_z, \hat{J}_\pm] &= \pm\hbar \hat{J}_\pm \\ [\hat{\vec{J}}^2, \hat{J}_\pm] &= 0 \end{aligned}}$$

(Übungsaufgabe 13.1)

Weitere Eigenschaften:

(1) $\hat{J}_\pm^+ = \hat{J}_\mp$

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

$\hat{J}_- \hat{J}_+ = \hat{\vec{J}}^2 - \hat{J}_z - \hbar \hat{J}_z$

$\hat{J}_\pm$ sind Leiteroperatoren bzgl. m in $|j,m\rangle$:

$$\hat{J}_z(\hat{J}_\pm |j,m\rangle) = (\hat{J}_\pm \hat{J}_z \pm \hbar \hat{J}_\pm)|j,m\rangle = \hbar(m\pm 1)(\hat{J}_\pm |j,m\rangle)$$

$$\Rightarrow \hat{J}_\pm |j,m\rangle \propto |j,m\pm 1\rangle$$

Normierung:

$$\begin{aligned} \| \hat{J}_\pm |j,m\rangle \|^2 &\overset{(1)}{=} \langle j,m| \hat{J}_\mp \hat{J}_\pm |j,m\rangle \\ &\overset{(2)}{=} \langle j,m| \hat{\vec{J}}^2 - \hat{J}_z^2 \mp \hbar \hat{J}_z |j,m\rangle \\ &= \hbar^2 j(j+1) - \hbar^2 m^2 \mp \hbar^2 m \end{aligned}$$

Also:

$$\boxed{\hat{J}_\pm |j,m\rangle = \hbar \sqrt{j(j+1) - m^2 \mp m}\; |j, m \pm 1\rangle}$$

Eigenwerte von $\hat{J}_z$ sind beschränkt:

$$\langle j,m | \hat{J}_x^2 + \hat{J}_y^2 | j,m\rangle = \langle j,m | \hat{J}^2 - \hat{J}_z^2 | j,m\rangle = \hbar^2 (j(j+1) - m^2) \geq 0$$

$$\Rightarrow |m| = \sqrt{j(j+1)}$$

$$\Rightarrow \exists\, m_{min}, m_{max} \in \mathbb{R}: \quad m_{min} \leq m \leq m_{max}$$

Eigenzustände zu m_{min} und m_{max}:

$$\hat{J}_+ |j, m_{max}\rangle = 0 \quad \overset{(2)}{\Rightarrow} \quad j(j+1) - m_{max}^2 - m_{max} = 0$$

$$\hat{J}_- |j, m_{min}\rangle = 0 \quad \overset{(2)}{\Rightarrow} \quad j(j+1) - m_{min}^2 + m_{min} = 0$$

$$\underset{m_{min} \leq m_{max}}{\Longrightarrow} \quad m_{min} = -j \quad \text{und} \quad m_{max} = +j$$

$$\Rightarrow \quad m = -j, -j+1, \dots, 0, \dots, +j-1, +j$$

$$\Rightarrow \quad 2j+1 \in \mathbb{N}$$

Also:

$$\boxed{\begin{aligned} j &= 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, \dots \\ m &= -j, -j+1, \dots, 0, \dots, j-1, j \end{aligned}}$$

Bemerkungen:

- Spektren von $\hat{J}_z$ und $\hat{\vec{J}}^2$ diskret
- Bahndrehimpuls $\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$: $j = \ell = 0, 1, 2, \ldots$ ganzzahlig
- Spin-Operator $\hat{\vec{S}}$ (Eigendrehimpuls) : $j = s = \begin{cases} \underset{\text{Higgs}}{0}, \underset{\text{Photon}}{1}, \underset{\text{Graviton}}{2}, \ldots & \text{Bosonen} \\ \underset{\text{Elektronen}}{\tfrac{1}{2}}, \tfrac{3}{2}, \ldots & \text{Fermionen} \end{cases}$

8.4 Spin $\frac{1}{2}$

Basisvektoren ($j = \frac{1}{2}$):

$$|j = \tfrac{1}{2}, m = \tfrac{1}{2}\rangle \equiv |\uparrow\rangle$$

$$|j = \tfrac{1}{2}, m = -\tfrac{1}{2}\rangle \equiv |\downarrow\rangle$$

Hilbert-Raum:

$\mathcal{H} = \text{lin}\{|\uparrow\rangle, |\downarrow\rangle\}$ 2-dimensional

Matrixelemente:

$$\langle \psi_i | \hat{A} | \psi_j \rangle = \begin{pmatrix} \langle \uparrow | \hat{A} | \uparrow \rangle & \langle \uparrow | \hat{A} | \downarrow \rangle \\ \langle \downarrow | \hat{A} | \uparrow \rangle & \langle \downarrow | \hat{A} | \downarrow \rangle \end{pmatrix}_{ij}$$ 2x2-Matrizen

Spin-Operator:

$$\hat{S}_i \underset{\substack{\uparrow \\ \text{Matrixdarstellung}}}{\hat{=}} \left(\langle \psi_i | \hat{S}_i | \psi_j \rangle \right) = \begin{pmatrix} \langle \uparrow | \hat{S}_i | \uparrow \rangle & \langle \uparrow | \hat{S}_i | \downarrow \rangle \\ \langle \downarrow | \hat{S}_i | \uparrow \rangle & \langle \downarrow | \hat{S}_i | \downarrow \rangle \end{pmatrix} =: S_i = \frac{\hbar}{2} \sigma_i$$

Pauli-Matrizen:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

mit

$$\sigma_i \sigma_j = \mathbb{1}_2 \delta_{ij} + i \varepsilon_{ijk} \sigma_k$$

Spin-Algebra:

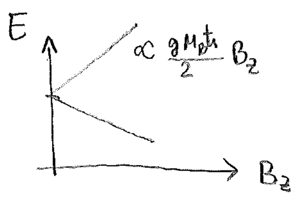
$$[S_i, S_j] = \left(\frac{\hbar}{2}\right)^2 \underbrace{[\sigma_i, \sigma_j]}_{2 i \varepsilon_{ijk} \sigma_k} = i \hbar \varepsilon_{ijk} S_k \quad ✓$$

$$\vec{S}^2 = \left(\frac{\hbar}{2}\right)^2 (\sigma_x^2 + \sigma_y^2 + \sigma_z^2) = \frac{3\hbar^2}{4} \mathbb{1}_2 = \hbar^2 j(j+1) \mathbb{1}_2 \quad \text{mit } j = \frac{1}{2} \quad ✓$$

Beispiel (Spin-$\frac{1}{2}$-Teilchen im Magnetfeld):

$$\hat{H}_{Zeeman} = -\vec{B} \cdot \hat{\vec{M}} = -B_z \hat{M}_z = g \mu_B B_z \hat{S}_z \underset{\substack{\uparrow \\ \text{Matrixdarstellung}}}{\hat{=}} \frac{g \mu_B \hbar}{2} B_z \sigma_z$$

für $\vec{B} \parallel \vec{e}_z$ und $\hat{M}_z = -\underset{\substack{\uparrow \\ g \approx 2}}{g} \underset{\substack{\uparrow \\ \text{Bohr-Magneton}}}{\mu_B} \hat{S}_z$ (magnetisches Moment).



$\Rightarrow$ Zeeman-Aufspaltung

8.5. Kugelflächenfunktionen

Eigenzustände des Bahndrehimpulsoperators:

$$\hat{\vec{L}}^2 |l,m\rangle = \hbar^2 l(l+1)\, |l,m\rangle$$

$$\hat{L}_z |l,m\rangle = \hbar m\, |l,m\rangle$$

mit $l = 0,1,2,\ldots$ und $m = -l, -l+1, \ldots, l-1, l$

Ortsdarstellung:

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

$$\hat{L}_\pm = \hat{L}_x \pm i \hat{L}_y \mathrel{\hat{=}} i\hbar\, e^{\pm i\varphi} \left(\cot\theta \frac{\partial}{\partial\varphi} \mp i \frac{\partial}{\partial\theta} \right)$$

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

Eigenfunktionen:

$$\boxed{Y_{lm}(\theta,\varphi) = \langle \vec{r} | l,m \rangle = \sqrt{\frac{2l+1}{4\pi}} \sqrt{\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta)\, e^{im\varphi}}$$

"Kugelflächenfunktionen"

Legendre-Polynome:

$$P_l^m(u) = \frac{(-1)^m}{2^l\, l!} (1-u^2)^{m/2} \frac{d^{l+m}}{du^{l+m}} (u^2-1)^l$$

Orthonormiertheit:

$$\int_0^{\pi} d\theta \sin\theta \int_0^{2\pi} d\varphi \; Y^*_{\ell m}(\theta,\varphi)\, Y_{\ell' m'}(\theta,\varphi) = \delta_{\ell\ell'}\,\delta_{mm'}$$

Vollständigkeit:

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\theta,\varphi)\, Y_{\ell m}(\theta',\varphi') = \delta(\varphi-\varphi')\,\delta(\cos\theta-\cos\theta')$$

⇒ Die Kugelflächenfunktionen bilden eine Orthonormalbasis auf dem Raum der normierbaren Funktionen $\psi = \psi(\theta,\varphi)$ auf der Kugeloberfläche (θ,φ).

Beispiele:

$\ell=0$: $\quad Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$

$\ell=1$: $\quad Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta$

$\quad Y_{1,\pm1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\varphi}$

$\ell=2$: $\quad Y_{20}(\theta,\varphi) = \sqrt{\frac{5}{16\pi}}\,(3\cos^2\theta-1)$

$\quad Y_{2,\pm1}(\theta,\varphi) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\varphi}$

$\quad Y_{2,\pm2}(\theta,\varphi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm i2\varphi}$

⋮

Eigenschaften:

- Parität: $Y_{lm}(\pi-\theta, \pi+\varphi) = (-1)^l Y_{lm}(\theta,\varphi)$

- Konjugation: $Y_{lm}^*(\theta,\varphi) = (-1)^m Y_{l,-m}(\theta,\varphi)$