Wiederholung

Heisenberg-Bild:

$$(\hat{q}_H)_{kn} = \langle u_k(\vec{x},t)|\hat{q}|u_n(\vec{x},t)\rangle$$

$$= \langle u_k(\vec{x})|e^{i\hat{H}t/\hbar}\,\hat{q}\,e^{-i\hat{H}t/\hbar}|u_n(\vec{x})\rangle$$

$$\Rightarrow \hat{q}_H = e^{i\hat{H}_s t/\hbar}\,\hat{q}_s\,e^{-i\hat{H}_s t/\hbar} \qquad (9.32)$$

L.S. bezieht sich auf Heisenberg-Basisfunktion, R.S. auf Schrödinger-Basisfunktionen.

$$(9.32) \Rightarrow \hat{H}_H = \hat{H}_S$$

Wechselwirkungs-Bild:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \quad , \quad \psi(\vec{x},t) = \sum_k \psi_k(t)\,u_k(\vec{x},t)$$

$$\hat{H}_0 u_k(\vec{x},t) = i\hbar\frac{\partial u_k}{\partial t}$$

$$\frac{d}{dt}\hat{q}_I = \frac{\partial \hat{q}_I}{\partial t} + \frac{i}{\hbar}(\hat{H}_{0I}, \hat{q}_I)$$

- Kontinuierlicher Index: $u_k, k \in \mathbb{Z} \rightarrow u_r, r \in \mathbb{R}^n$

$$\sum_k \rightarrow \int dr \quad , \quad \delta_{kk'} \rightarrow \delta(r-r')$$

- Drehimpuls $\hat{L} = \hat{x} \times \hat{p}$ eindeutig

$$[\hat{L}_z, \hat{a}_z] = 0 \quad , [\hat{L}_z, \hat{a}_x] = i\hbar\,\hat{a}_y \quad , \quad [\hat{L}_z, \hat{a}_y] = -i\hbar\,\hat{a}_x$$

wobei $\hat{a} = \hat{x}$ oder $\hat{p}$

$$[\hat{L}_z, \hat{L}_x] = i\hbar\, \hat{L}_y \qquad (10.6a)$$

$$[\hat{L}_z, \hat{L}_y] = i\hbar\, \hat{L}_x \qquad (10.6b)$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar\, \hat{L}_z \qquad (10.6c)$$

Ebenfalls nützlich: Quadrant des Bahn-Drehimpulses

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \qquad (10.7)$$

$$\Rightarrow [\hat{L}^2, \hat{L}_x] = [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x]$$

$$\underset{(\ddot{U}6.1)}{=} \hat{L}_y[\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x]\hat{L}_y + \hat{L}_z[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z$$

$$\underset{(10.6)}{=} i\hbar(-\hat{L}_y\hat{L}_z - \hat{L}_z\hat{L}_y + \hat{L}_z\hat{L}_y + \hat{L}_y\hat{L}_z)$$

$$= 0 = [\hat{L}^2, \hat{\vec{L}}] \qquad (10.8)$$

$\Rightarrow \exists$ Funktion ψ, die Eigenfunktion von $\hat{L}_z$ und $\hat{L}^2$ sind

$$\hat{L}^2\psi = a\psi \;, \quad \hat{L}_z\psi = b\psi \qquad a, b \in \mathbb{R} \qquad (10.9)$$

$$(10.7) \Rightarrow \langle \hat{L}^2 \rangle \geq \langle \hat{L}_z^2 \rangle \Rightarrow a \geq b^2 \qquad (10.10)$$

Einführe Auf-und-Absteige-Operatoren (→ Kap. 6.6)

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y \qquad (10.11)$$

$$(\hat{L}_\pm)^\dagger = \hat{L}_\mp \qquad (10.12)$$

$$\hat{L}_\pm \hat{L}_\mp = (\hat{L}_x \pm i\hat{L}_y)(\hat{L}_x \mp i\hat{L}_y)$$

$$= \hat{L}_x^2 + \hat{L}_y^2 \pm i(\underbrace{\hat{L}_y\hat{L}_x - \hat{L}_x\hat{L}_y}_{= i\hbar\hat{L}_z}) = \hat{L}_x^2 + \hat{L}_y^2 \pm \hbar\hat{L}_z \qquad (10.13)$$

$$[\hat{L}_z, \hat{L}_\pm] = [\hat{L}_z, \hat{L}_x] \pm i[\hat{L}_z, \hat{L}_y] = i\hbar \hat{L}_y \pm \hbar \hat{L}_x$$
$$= \pm\hbar(\hat{L}_x \pm i\hat{L}_y) = \pm\hbar \hat{L}_\pm$$
$$\Rightarrow \hat{L}_z \hat{L}_\pm \psi = (\hat{L}_\pm \hat{L}_z + [\hat{L}_z, \hat{L}_\pm])\psi$$
$$= (\hat{L}_\pm b \pm \hbar \hat{L}_\pm)\psi$$
$$\Rightarrow \hat{L}_z \hat{L}_\pm \psi = (b \pm \hbar)\hat{L}_\pm \psi \qquad (10.15)$$

$\hat{L}_\pm \psi$ ist selber Eigenfunktion vo $\hat{L}_z$, mit erhöhtem ($\hat{L}_+$), bzw. reduziertem ($\hat{L}_-$) Eigenwert.

$(10.8) \Rightarrow [\hat{L}^2, \hat{L}_\pm] = 0 \quad \Rightarrow \hat{L}^2(\hat{L}_\pm \psi) = a \hat{L}_\pm \psi$

Eigenwert von $\hat{L}^2$ unverändert.

$(10.10) \Rightarrow$ "Die Leiter muss enden": $\exists$ Eigenfunktion ψ_+ zu $\hat{L}^2$ und $\hat{L}_z$, so dass $\hat{L}_+ \psi_+ = 0$ (10.16)
Dies ist Eigenfunktion mit größtmöglichem $b = b_{max}$, für festes a:

$$\hat{L}_z \psi_+ = b_{max} \psi_+$$
$$\hat{L}_- \hat{L}_+ \psi_+ \overset{(10.16)}{=} 0$$
$$\hookrightarrow_{\overset{=}{(10.13)}} (\hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z)\psi_+ = (a - b_{max}^2 - \hbar b_{max})\psi_+$$

$$\Rightarrow a = b_{max}(b_{max} + \hbar^2) \qquad (10.18)$$

$$\hat{L}_z (\hat{L}_-)^n \psi_+ = (b_{max} - n\hbar)(\hat{L}_-)^n \psi_+ \qquad (10.19)$$

(10.10) : $\exists$ Eigenfunktion $\psi_- = (\hat{L}_-)^{n_{max}} \psi_+$ mit <u>kleinstem</u> Eigenwert von $\hat{L}_z$, mit $\hat{L}_- \psi_- = 0$

$$\Rightarrow \hat{L}_+ \hat{L}_- \psi_- = 0$$

$$\hookrightarrow = (\hat{L}^2 - \hat{L}_z^2 + \hbar \hat{L}_z) \psi_-$$

$$= [a - (b_{max} - n_{max}\hbar)^2 + \hbar (b_{max} - n_{max}\hbar)] \psi_-$$

$$\Rightarrow a = (b_{max} - n_{max}\hbar)^2 - \hbar (b_{max} - n_{max}\hbar) \qquad (10.21)$$

(10.18), (10.21)

$$\Rightarrow b_{max}(b_{max} + \hbar) = (b_{max} - n_{max}\hbar)^2 - \hbar (b_{max} - n_{max}\hbar)$$

$$= b_{max}^2 - 2 b_{max} n_{max} \hbar + n_{max}^2 \hbar^2$$

$$- \hbar b_{max} + n_{max} \hbar^2$$

$$\Rightarrow -2 b_{max}(1 + n_{max}) + n_{max}\hbar \underbrace{(1 + n_{max})}_{\neq 0} = 0$$

$$\Rightarrow \quad b_{max} = \frac{n_{max}}{2} \hbar \qquad (10.22)$$

$b_{max} = \ell \hbar$ $\qquad$ ℓ: ganz- oder halbzahlig

Später: Für Bahndrehimpulse: nur $\ell \in \mathbb{N}^0$ erlaubt

(10.9) $\Rightarrow$

$$\hat{L}^2 \psi_{lm} = \hbar^2 \ell(\ell+1) \psi_{lm}, \quad l = 0, 1, 2, \ldots \qquad (10.23a)$$

$$\hat{L}_z \psi_{lm} = \hbar m \psi_{lm}, \quad m = -\ell, -\ell+1, \ldots, 0, \ldots, \ell-1, \ell \qquad (10.23b)$$

10b Wiederholung: Kugel- und Zylinderkoordinaten

Falls System volle (3-dim) Rotationssymmetrie besitzt:
Benutzung von <u>Kugelkoordinaten</u> oft vorteilhaft:

$$x = r\sin\theta\cos\varphi \quad , y = r\sin\theta\sin\varphi \quad , \quad z = r\cos\theta \qquad (10.24)$$

mit $r \in [0, \infty]$, $\theta \in [0, \pi]$, $\varphi \in [0, 2\pi]$

$\Rightarrow \cos\theta \in [-1, 1]$, $\sin\theta \in [0, 1]$

Inversion:

$$r = \sqrt{x^2+y^2+z^2}, \quad \varphi = \arctan\frac{y}{x} \quad , \theta = \arctan\frac{\sqrt{x^2+y^2}}{z} \qquad (10.25)$$

Volumenintegral:

$$\int d^3x = \int_{-\infty}^{\infty} dx \int dy \int dz = \iiint dr\, d\theta\, d\varphi \left| \frac{\partial(x,y,z)}{\partial(r,\theta,\varphi)} \right|$$

$$= \int_0^{\infty} dr\, r^2 \int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta) \qquad (10.26)$$

Ableitungen

$$\left.\begin{aligned}
\frac{\partial}{\partial x} &= \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial x}\frac{\partial}{\partial\varphi} \\
&= \sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi} \\
\frac{\partial}{\partial y} &= \sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi} \\
\frac{\partial}{\partial z} &= \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}
\end{aligned}\right\} \qquad (10.27)$$

$$\Rightarrow \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$= \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial \theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin\theta}\frac{\partial^2}{\partial\varphi^2}\right) \qquad (10.28)$$

<u>Zylinder Koordinaten</u> sind nützlich, falls System invariant unter Rotation um z-Achse ist.

$$x = r\cos\varphi \,, \quad y = r\sin\varphi \,, \quad z = z \qquad (10.29)$$

$$r \in [0, \infty] \,, \ \varphi [0, 2\pi] \,, \ z \in [0, \infty]$$

$$\Rightarrow r = \sqrt{x^2+y^2} \,, \quad \varphi = \arctan\frac{y}{x} \,, \quad z = 7 \qquad (10.30)$$

$$\iint dx\,dy = \int_0^\infty r\,dr \int_0^{2\pi} d\varphi \qquad (10.31)$$

$$\left.\begin{aligned} \frac{\partial}{\partial x} &= \cos\varphi\frac{\partial}{\partial r} - \frac{\sin\varphi}{r}\frac{\partial}{\partial\varphi} \\ \frac{\partial}{\partial y} &= \sin\varphi\frac{\partial}{\partial r} + \frac{\cos\varphi}{r}\frac{\partial}{\partial\varphi} \end{aligned}\right\} \qquad (10.32)$$

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi} + \frac{\partial^2}{\partial z^2} \qquad (10.33)$$

10c Eigenfunktionen des Bahndrehimpulses

Benutze Kugelkoordinaten!

$$\hat{L}_z \underset{(10.4c)}{=} -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

$$\underset{(10.24,27)}{=} -i\hbar\Big[r\sin\theta\cos\varphi\left(\sin\theta\sin\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\sin\varphi}{r}\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\right)$$

$$-r\sin\theta\sin\varphi\left(\sin\theta\cos\varphi\frac{\partial}{\partial r} + \frac{\cos\theta\cos\varphi}{r}\frac{\partial}{\partial\theta} + \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}\right)\Big]$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi} \qquad (10.34)$$

$\Rightarrow$ Eigenfunktion von $\hat{L}_z$ hängen nur von φ ab!

$\hat{L}_z \psi_{lm} = \hbar m \psi_{lm}$

$$\Rightarrow \psi_{lm}(r,\theta,\varphi) = e^{im\varphi} F_{lm}(r,\theta) \qquad (10.35)$$

Wellen $\psi_{lm}(r,\theta,0) = \psi_{lm}(r,\theta,2\pi)$

$\Rightarrow$ m ist ganzzahlig!

Analog:
$$\left.\begin{aligned}\hat{L}_x &= -i\hbar\left(-\sin\varphi\frac{\partial}{\partial\theta} - \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)\\ \hat{L}_y &= -i\hbar\left(\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)\end{aligned}\right\} \qquad (10.36)$$

$\hat{L}$ enthält nur Ableitungen nach θ, φ, kein $\frac{\partial}{\partial r}$

$\Rightarrow F_{lm}(r,\theta) = f_{lm}(\theta)\, g(r)$

$$\hat{L}_\pm \underset{(10.11)}{=} \hat{L}_x \pm i\hat{L}_y \underset{(10.36)}{=} -i\hbar\Big[(-\sin\varphi \pm i\cos\varphi)\frac{\partial}{\partial\theta}$$

$$-\cot\theta(\cos\varphi \pm i\sin\varphi)\frac{\partial}{\partial\varphi}\Big]$$

$$= \hbar\left[\pm(\pm i\sin\varphi + \cos\varphi)\frac{\partial}{\partial\theta} + i\cot\theta\, e^{\pm i\varphi}\frac{\partial}{\partial\varphi}\right]$$

$$= \hbar e^{\pm i\varphi}\left(\pm\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) = \hat{L}_\pm \qquad (10.37)$$

$$\hat{L}_+ \hat{L}_- = \hbar^2 e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right)e^{-i\varphi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right)$$

$$= \hbar^2 e^{i\varphi}\Big[e^{-i\varphi}\left(-\frac{\partial^2}{\partial\theta^2} - \frac{1}{\sin^2\theta}\frac{\partial}{\partial\varphi} + i\cot\theta\frac{\partial^2}{\partial\theta\partial\varphi}\right)$$

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

$$+ ie^{-i\varphi}\cot\theta\left(-\frac{\partial^2}{\partial\varphi\partial\theta} + i\cot\theta\frac{\partial^2}{\partial\varphi^2}\right)\Big]$$

$$= \hbar^2\left(-\frac{\partial^2}{\partial\theta^2} + i\frac{\cos^2\theta - 1}{\sin^2\theta}\frac{\partial}{\partial\varphi} - \cot\theta\frac{\partial}{\partial\theta} - \cot^2\theta\frac{\partial^2}{\partial\varphi^2}\right)$$

$$\Rightarrow \hat{L}_+ \hat{L}_- = -\hbar^2\left(+i\frac{\partial}{\partial\varphi} + \cot\theta\frac{\partial}{\partial\theta} + \frac{\partial^2}{\partial\theta^2} + \cot^2\theta\frac{\partial^2}{\partial\varphi^2}\right) \quad (10.38)$$