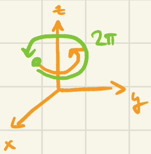
Review: Eigenfunctions of angular momentum operator

$$\langle \theta, \varphi | l, m \rangle \equiv Y_l^m(\theta,\varphi)$$

with $\hat{\vec{L}}$ in polar coordinates



$$\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi} = \hat{p}_\varphi$$

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

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

independent of r

Explicit eigenfunctions $\longrightarrow$ separation ansatz

$$Y_l^m(\theta,\varphi) = \Phi_m(\varphi)\,\Theta_l^m(\theta)$$

$\hat{L}_z \Phi_m(\varphi) = m\hbar\,\Phi_m(\varphi)$ $\longrightarrow$ $= e^{im\varphi}\,\Theta_l^m(\theta)$

$\hookrightarrow$ $l = 0,1,2,\dots$ integer only for orbital ang. mom.

$(\hat{L}_- Y_l^{-l} = 0)$ $\quad \hat{L}_+ Y_l^l = 0 \Rightarrow \Theta_l^l(\theta) = \text{const.}\,(\sin\theta)^l \rightarrow Y_l^l \sim e^{il\varphi}(\sin\theta)^l$

$$Y_l^{l-k} \sim (\hat{L}_-)^k\, Y_l^l \quad , \quad k = 1,\dots,2l$$

$$\Rightarrow \quad Y_l^m(\theta,\varphi) = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\,(-1)^m\, e^{im\varphi}\, P_l^m(\cos\theta)$$

mit assoziiertem Legendrepolynom P_l^m

$$P_l^m = (-1)^l \frac{1}{2^l\, l!}(\sin\theta)^m\left(\frac{d}{d\cos\theta}\right)^{l+m}(\sin\theta)^{2l}$$

Spezialfall $m=0$: $Y_\ell^0(\theta,\varphi) = \sqrt{\frac{2\ell+1}{4\pi}} \underbrace{P_\ell(\cos\theta)}_{\text{normales Legendre Polynom}}$

unabh. von φ

$$\underbrace{\hat{L}_z}_{=\frac{\hbar}{i}\frac{\partial}{\partial\varphi}} Y_\ell^m(\theta,\varphi) = m\hbar\, Y_\ell^m(\theta,\varphi)$$

$$\underbrace{\hat{\vec{L}}^2}_{=-\hbar^2(\cdots\cdots)} Y_\ell^m(\theta,\varphi) = \ell(\ell+1)\hbar^2\, Y_\ell^m(\theta,\varphi)$$

Beispiele: $Y_0^0(\theta,\varphi) = \sqrt{\frac{1}{4\pi}} = \frac{1}{\sqrt{O}}$ $\quad O =$ Oberfläche der Einheitskugel

$\ell = 1$

$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$ $\qquad P_1(\cos\theta) = \cos\theta$

$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\, e^{i\varphi} \sin\theta$

$Y_1^{-1} = +\sqrt{\frac{3}{8\pi}}\, e^{-i\varphi} \sin\theta$

Y_ℓ^m: Kugelflächenfunktion $\longrightarrow$ Satz vollst. Funktion auf Einheitskugel

$\longrightarrow \Psi(\vec{r}) = R(r)\, Y_\ell^m(\theta,\varphi)$ $\circledast$

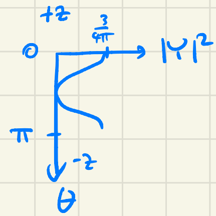
Normierung: $\langle \ell m | \ell' m' \rangle \overset{!}{=} \delta_{\ell\ell'} \delta_{mm'}$

$$= \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\varphi\, \langle \ell m | \theta\varphi \rangle \langle \theta\varphi | \ell' m' \rangle$$

$$\Rightarrow \underbrace{\int_{-1}^{1} d\cos\theta}_{\int_0^\pi \sin\theta \, d\theta} \int_0^{2\pi} d\varphi \, \left(Y_\ell^m(\theta,\varphi)\right)^* Y_{\ell'}^{m'}(\theta,\varphi) = \delta_{\ell\ell'}\,\delta_{mm'}$$

$$(*) \Rightarrow \quad |\psi(\vec r)|^2 = |R(r)|^2 \, \underbrace{|Y_\ell^m(\theta,\varphi)|^2}_{\frac{3}{4\pi}\cos^2\theta}$$

Beispiel $\ell = 1$, $m = 0$



- Eigenschaften der Kugelflächenfkten ✓
- Sphärisch sym. Potentiale und radiale S-Glg.

Eigenschaften

1) $$\left(Y_\ell^m\right)^* = (-1)^m \, Y_\ell^{-m}$$ (Konvention)

Spezialfall: $\left(Y_\ell^\ell\right)^* = (-1)^\ell \, Y_\ell^{-\ell}$

$$\rightarrow \left(\hat L_+ Y_\ell^\ell\right)^+ = 0 = \hat L_- Y_\ell^{-\ell}$$

$$\hat L_- Y_\ell^{\ell *} = 0 = \hat L_- Y_\ell^{-\ell}$$

2) Verhalten von Y_ℓ^m unter Parität/Raumspiegelung

$$\vec r \to -\vec r \iff \varphi \to \varphi + \pi, \quad \theta \to \pi - \theta$$

$$Y_\ell^m(\pi-\theta, \varphi+\pi) = (-1)^\ell \, Y_\ell^m(\theta,\varphi)$$

$$\downarrow \qquad \downarrow$$

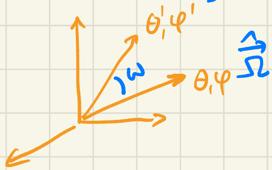
$$(-1)^{\ell+m} \qquad (-1)^m$$

Parität $(-1)^\ell$ gerade oder ungerade entsprechend ℓ gerade oder ung.
unabh. von m

3) Additionstheorem der Kugelflächenfunktionen

$$\frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} \left(Y_\ell^m(\theta',\varphi')\right)^* Y_\ell^m(\theta,\varphi) = P_\ell(\cos\omega)$$

$\hat{\vec{\Omega}}'$



mit $\cos\omega = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi-\varphi')$
d.h. $\omega = \sphericalangle(\hat{\vec{\Omega}}, \hat{\vec{\Omega}}')$

4) Vollständigkeit auf Einheitskugel

$\langle\theta'\varphi'| \quad |\theta\varphi\rangle$

$$\mathbb{1} = \sum_{\ell,m} |\ell m\rangle\langle \ell m|$$

$$\Rightarrow \delta(\cos\theta - \cos\theta')\,\delta(\varphi-\varphi') = \sum_{\ell m} \langle\theta'\varphi'|\ell m\rangle\langle \ell m|\theta,\varphi\rangle$$

$$= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta',\varphi')\left(Y_\ell^m(\theta,\varphi)\right)^*$$

Sphärisch symmetrische Potentiale

$$[\hat{H}, \hat{\vec{L}}] = 0$$

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

$$\hat{H} = \underbrace{\frac{\hat{\vec{p}}^2}{2m}}_{?} + \underbrace{V(|\hat{\vec{r}}|)}_{V(r)}$$ mit sphärisch sym. lokalen Potential $V(|\vec{r}|)$

Laplaceoperator $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ in Polarkoordinaten?

$\rightarrow$ Kettenregel HW

$$\Rightarrow \boxed{\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\hat{\vec{L}}^2}$$

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

oder $$\boxed{\Delta = \left(\frac{1}{r}\frac{\partial}{\partial r}\cdot r\right)^2 - \frac{\hat{\vec{L}}^2}{\hbar^2 r^2}}$$

$$\vec{p}^2 = -\hbar^2\Delta = \underbrace{\left(\frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r} r\right)^2}_{\hat{p}_r^2} + \underbrace{\frac{\vec{L}^2}{r^2}}_{\hat{\vec{p}}_\Omega^2}$$

$\Rightarrow$ Schrödingergl. für $V(r)$ (sphärisch sym.)

$$\big(\underbrace{\hat{T}_r + \overbrace{\hat{T}_\Omega}^{\hat{H}_\Omega} + \hat{V}(r)}_{\hat{H}_r}\big)\,\Psi_E(r,\theta,\varphi) = E\,\Psi_E(r,\theta,\varphi)$$

Separationsansatz $\Psi_E(r,\theta,\varphi) = R_E(r)\, W(\theta,\varphi)$

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{\vec{L}}^2}{2mr^2} + V(r)\right)\Psi_E = E\,\Psi_E$$

$\rightarrow$ W ist Eigenfkt. von $\hat{\vec{L}}^2$, $W = Y_\ell^m$

$$\Rightarrow \quad \Psi_{E,\ell,m}(r,\theta,\varphi) = R_{E,\ell,\cancel{m}}(r)\, Y_\ell^m(\theta,\varphi)$$

in S-Glg.

$$\Rightarrow \left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\underbrace{\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)}_{r u''} + \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r)\right) R_{E,\ell}(r) = E\, R_{E,\ell}(r)$$

Für V(r) reduziert sich 3d S-Glg. zu 1d. Diffglg. in r

Transformation: $R_{E\ell}(r) = \dfrac{u_{E\ell}(r)}{r}$

$$\Rightarrow \quad R' = \frac{u'}{r} - \frac{u}{r^2}$$

$$\Rightarrow \quad r^2 R' = r\cdot u' - u$$

$$\Rightarrow \quad \left(r^2 R'\right)' = u' + r u'' - u' = r\, u''$$

$$\Rightarrow \boxed{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r)\right) u_{E\ell}(r) = E\, u_{E,\ell}(r)}$$

$\rightarrow$ Radiale Schrödingergleichung für $u_{E\ell}(r)$

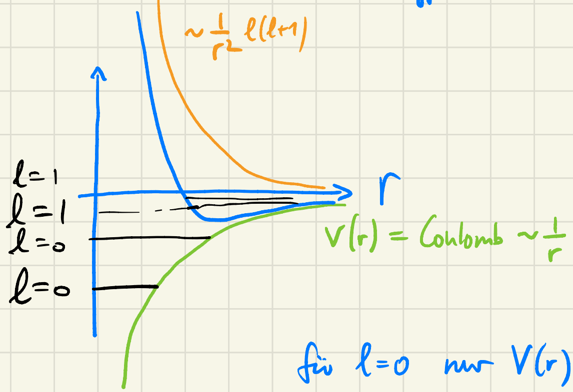
mit Normierung $\displaystyle\int |\Psi_E|^2 d^3r = \underbrace{\int_0^{2\pi} d\varphi \int_{-1}^{1} d\cos\theta\, |Y_\ell^m|^2}_{=1} \int_0^\infty \cancel{r^2}\, dr\, \frac{|u_{E\ell}(r)|^2}{\cancel{r^2}}$

Lösung der rad. S-Glg. $u_{E,l}(r)$ hat Normierung $\int_0^\infty dr\, |u_{E,l}(r)|^2 = 1$

→ Radiale S-Glg. ist äquivalent zu 1d S-Glg.

in effektivem Potential $V_{eff}(r) = V(r) + \underbrace{\frac{l(l+1)\hbar^2}{2mr^2}}$

abstoßendes Zentrifugalpot.
vgl. Theo I



für $l=0$ nur $V(r)$

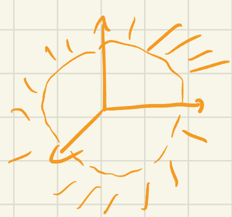
Randbedingung: Da $R_{E,l} = \frac{u_{E,l}}{r} \Rightarrow u_{E,l}(r \to 0) \to 0$

außer für bei $r=0$ sing. Pot.
$V \sim \delta(\vec{r})$

Einfache Probleme

1) freie Teilchen (in Polarkoord.)

2) unendl. sphärischer Potentialkasten



3) endl. sphärischer attraktiver Pot.topf

4) sphärisch sym. HO || 9. Wasserstoffatom