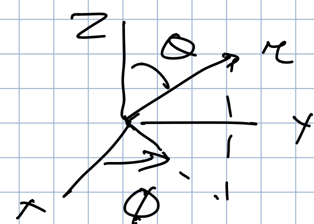
⟹ VORLESUNG 16 QM

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(\bar{r}) = E\,\psi(\bar{r})$$

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

$r,\ \theta,\ \phi$



$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right] + V(r)\psi = E\psi$$

$$\psi(\bar{r}) = R(r)\,Y(\theta,\phi)$$

$$\frac{Y}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{2m}{\hbar^2}\left(V(r) - E\right)YR$$

$$+ R\left[\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = 0$$

$$\frac{r^2}{YR}$$

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{2mr^2}{\hbar^2}\left(V(r) - E\right)$$

$$+\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = 0$$

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - \frac{2mr^2}{\hbar^2}\left(V(r) - E\right) = \ell(\ell+1)$$

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

m

$$Y(\theta,\phi) = Y_{\ell m}(\theta,\phi)$$

$$= C\, e^{im\phi}\, P_\ell^m(\cos\theta)$$

$$\int d\Omega\, |Y(\theta,\phi)|^2 = 1$$

$$d\Omega = \sin\theta \, d\theta \, d\phi$$

$$\psi(\bar{r}) = R(r) \, Y_{\ell m}(\theta, \phi)$$

$$R(r) = \frac{U(r)}{r}$$

$$\frac{\partial R}{\partial r} = -\frac{U}{r^2} + \frac{1}{r}\frac{dU}{dr}$$

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial R}{\partial r}\right) = \frac{d}{dr}\left(-U + r\frac{dU}{dr}\right)$$

$$= -\cancel{\frac{dU}{dr}} + \cancel{\frac{dU}{dr}} + r\frac{d^2U}{dr^2}$$

$$\cancel{r}\,\frac{d^2U}{dr^2} - \frac{2m\cancel{r^2}}{\hbar^2}\left[V(r) - E\right]\frac{U}{\cancel{r^2}} = \ell(\ell+1)\frac{U}{r^2}$$

$$\times\left(-\frac{\hbar^2}{2m}\right)$$

$$-\frac{\hbar^2}{2m}\frac{d^2U}{dr^2} + \left[V(r) + \underbrace{\frac{\hbar^2\ell(\ell+1)}{2mr^2}}\right]U = EU$$

REPULSIVE

ZENTRIFUGAL POTENTIAL

$$L^2 \rightsquigarrow \hbar^2 \ell(\ell+1)$$

$$V_{eff}(r) \equiv V(r) + \frac{\hbar^2 \ell(\ell+1)}{2 m r^2}$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2 u}{dr^2} + V_{eff}(r)\, u = E\, u$$

$$\underline{\ell = 0} \qquad V_{eff} = V$$

NORMIERUNG

$$\int d^3\bar{r}\; |\psi(\bar{r})|^2 = 1$$

$$\int dr\, r^2 \underbrace{\int d\theta \sin\theta \int d\phi}_{\int d\Omega}\; |R|^2\, |Y|^2 = 1$$

$$d\Omega = d\cos\theta\; d\phi$$

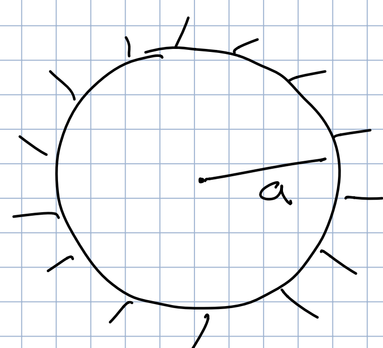
$$\int dr\, r^2 |R|^2 \underbrace{\int d\Omega\, |Y|^2}_{1} = 1$$

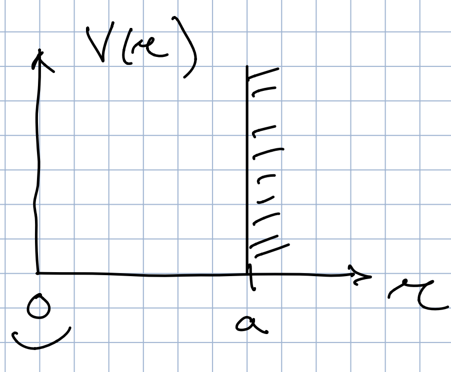
$$\int dr \; r^2 \; |R|^2 = 1$$

$$R(r) = \frac{U(r)}{r}$$

$$\int_0^\infty dr \; |U(r)|^2 = 1$$

$\Rightarrow$ UNENDLICHE SPHERISCHER POTENTIALTOPF





$$r \geq a \qquad U(r) = 0$$

$r < a$

$$\Longrightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\,u = E\,u$$

$$\Longrightarrow \quad \boxed{\ell = 0}$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} = E\,u$$

$$\rightsquigarrow E = \frac{\hbar^2}{2m}k^2$$

$$\frac{d^2u}{dr^2} = -k^2 u$$

$$u(r) = A\sin(kr) + B\cos(kr)$$

- $r = 0$

$$\psi = R\,Y_{00}$$

$$= \frac{u}{r}\,Y_{00}$$

$$\frac{\sin(kr)}{r} \xrightarrow[r\to 0]{} k$$

$$\frac{\cos(kr)}{r} \longrightarrow \infty$$

$$\longrightarrow \underline{\underline{B = 0}}$$

$$U(r) = A \sin(kr)$$

- $\underline{\underline{r = a}}$ $\qquad U(a) = 0$

$$ka = n\pi \qquad n = 1, 2, 3, \ldots$$

$$U(r) = A \sin\left(\frac{n\pi}{a} r\right)$$

$$l = 0 \quad \begin{cases} R_n(r) = \dfrac{A}{r} \sin\left(\dfrac{n\pi}{a} r\right) \\[2ex] E_n = \dfrac{\hbar}{2m} \left(\dfrac{n\pi}{a}\right)^2 \end{cases}$$

$$A \Longrightarrow \int_0^a dr \, |U(r)|^2 = 1$$

$$\downarrow$$

$$A^2 \underbrace{\int_0^a dr \, \sin^2\left(\frac{n\pi}{a} r\right)}_{a\left(\frac{1}{2}\right)} = 1$$

$$A = \sqrt{\frac{2}{a}}$$

$$\psi = R_n Y_{00} \rightarrow \frac{1}{\sqrt{4\pi}}$$

$$\boxed{\psi_{n00} = \sqrt{\frac{2}{a}}\ \frac{1}{r}\ \sin\left(\frac{n\pi}{a} r\right)\ \frac{1}{\sqrt{4\pi}}}$$

ℓ m

$\Longrightarrow$ ALLGEMEINES ℓ

$$\rightsquigarrow\ -\frac{d^2 u}{dr^2} + \frac{\ell(\ell+1)}{r^2}\, u = k^2 u$$

$$R(r) = \frac{u(r)}{r} = A\, j_\ell(kr) + \cancel{B\, n_\ell(kr)}$$

SPHERISCHE

BESSEL NEUMANN

FUNKTIONEN

$$j_\ell(x) = (-1)^\ell x^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin x}{x}$$

$$n_\ell(x) = (-1)^{\ell+1} x^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos x}{x}$$

$$j_0(x) = \frac{\sin x}{x}$$

$$n_0(x) = -\frac{\cos x}{x}$$

$$j_1(x) = -\cancel{x}\left(\frac{1}{\cancel{x}}\frac{d}{dx}\right)\frac{\sin x}{x}$$

$$= \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

$$\xrightarrow[x \to 0]{} \frac{1}{x^2}\left(\cancel{x} - \frac{x^3}{3!}\right) - \frac{1}{x}\left(\cancel{1} - \frac{x^2}{2!}\right) + \dots$$

$$= x\left(\frac{1}{2} - \frac{1}{6}\right) = \frac{x}{3}$$

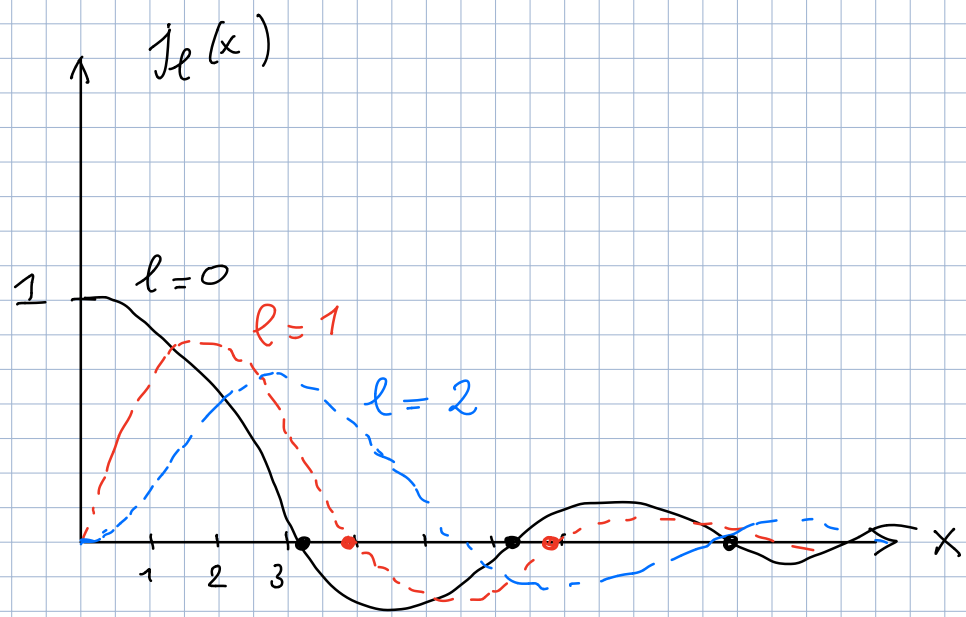
$$n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

$$n_1(x) \xrightarrow[x \to 0]{} \infty$$

$$j_\ell(x) \xrightarrow[x \to 0]{} \frac{x^\ell}{(2\ell+1)!!}$$

$$n!! = n(n-2)\dots 1$$

$\underline{\ell = 1}$ $\qquad 3!! = 3 \cdot 1$



$$R(r) = A \, j_\ell(kr)$$

$\underline{r = a}$ $\qquad j_\ell(ka) = 0$

$\beta_{n\ell}$ NULLSTELLEN $j_\ell(kr)$

$n = 1, 2, \dots$

$$ka = \beta_{n\ell}$$

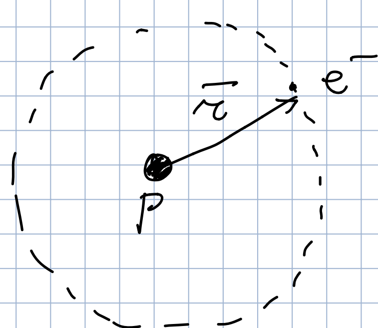
$$k = \frac{1}{a} \beta_{n\ell} \Rightarrow \boxed{E_{n\ell} = \frac{\hbar^2}{2m} \frac{1}{a^2} \beta_{n\ell}^2}$$

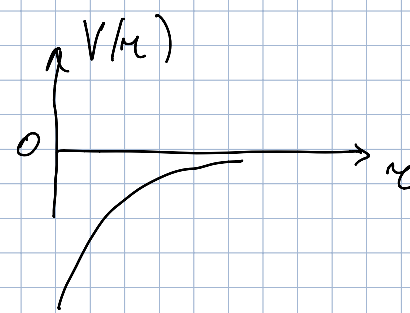
$$\psi_{n\ell m}(\vec{r}) = A_{n\ell}\, j_\ell\left(\beta_{n\ell}\frac{r}{a}\right) Y_{\ell m}(\theta,\phi)$$

$$\int d^3r\, |\psi|^2 = 1$$

$$\int_0^\infty dr\, r^2\, \underline{\underline{A_{n\ell}^2}}\, j_\ell^2\left(\beta_{n\ell}\frac{r}{a}\right) = 1$$

$\Rightarrow$ 4.2 H - ATOM





COULOMB POT.

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r} = -\alpha\frac{\hbar c}{r}$$

$$\alpha \equiv \left(\frac{e^2}{4\pi\varepsilon_0 \hbar c}\right) \simeq \frac{1}{137}$$

OHNE DIMENSION

FEINSTRUKTUR KONSTANTE

$$[\hbar c] : \quad Js\,\frac{m}{s}$$

$$\hbar c \simeq (197)\ \text{MeV fm}$$

$$1\ \text{MeV} = 10^{6}\ \text{eV}$$

$$1\ \text{fm} = 10^{-15}\ m$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[-\alpha\frac{\hbar c}{r} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u = E\,u$$

$E < 0 \implies$ GEBUNDENE ZUSTÄNDE

$$E = -\frac{\hbar^2}{2m}K^2$$

$$\frac{d^2u}{dr^2} = \underline{\underline{K^2}}\,u - \frac{2m}{\hbar^2}\frac{\alpha\hbar c}{r}\,u + \frac{\ell(\ell+1)}{r^2}\,u$$

$$\frac{1}{K^2} \qquad E = -\frac{\hbar^2 c^2}{2mc^2}K^2$$

$$[K] = \frac{1}{m}$$

$\rho \equiv \kappa r$ OHNE DIMENSION

$$\frac{d^2 u}{d\rho^2} = \left[1 - \underbrace{\frac{2m}{\hbar^2} \frac{\alpha \hbar c}{\kappa}}_{\equiv \rho_0} \frac{1}{\rho} + \frac{\ell(\ell+1)}{\rho^2} \right] u$$

$$\frac{d^2 u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2} \right] u$$