Teilchen im Zentralpotenzial

$$\boxed{H = \frac{|\vec{p}|^2}{2m} + V(|\vec{r}|)}$$

$\Rightarrow$ Kugelkoordinaten: r, ϑ, φ

$$|\vec{p}|^2 = -\hbar^2 \Delta \stackrel{!}{=} -\frac{\hbar^2}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}$$

$$\frac{1}{r^2}\Bigg(\underbrace{-\hbar^2\left(\frac{1}{\sin\vartheta} \frac{\partial}{\partial\vartheta} \sin\vartheta \frac{\partial}{\partial\vartheta} + \frac{1}{\sin^2\vartheta} \frac{\partial^2}{\partial\varphi^2}\right)}_{L^2}\Bigg)$$

$\rightarrow$ stat. Sch.-gl.: $\psi = \psi(r, \vartheta, \varphi)$

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

$\rightarrow$ Rotationsvarianz:

$$[H, L^2] = 0, \quad [H, L_3] = 0$$

$$\left([L^2, L_3] = 0\right)$$

gemeinsame Eigenzustände:

$$|E, l, m\rangle \longrightarrow \psi(r,\vartheta,\varphi) = \langle \vec{x}|E,l,m\rangle$$

der Op H, L^2, L_3 zu EWen $E, \hbar^2 l(l+1)$ und $\hbar m$:

→ <u>Ansatz</u>:

$$\psi(r,\vartheta,\varphi) = \frac{u(r)}{r} Y_{l,m}(\vartheta,\varphi)$$

$$\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\left(\frac{u}{r}\right) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(-u + r u'\right)$$

$$= \frac{1}{r} u''$$

- $L^2 Y_{l,m} = \hbar^2 l(l+1) Y_{l,m}$

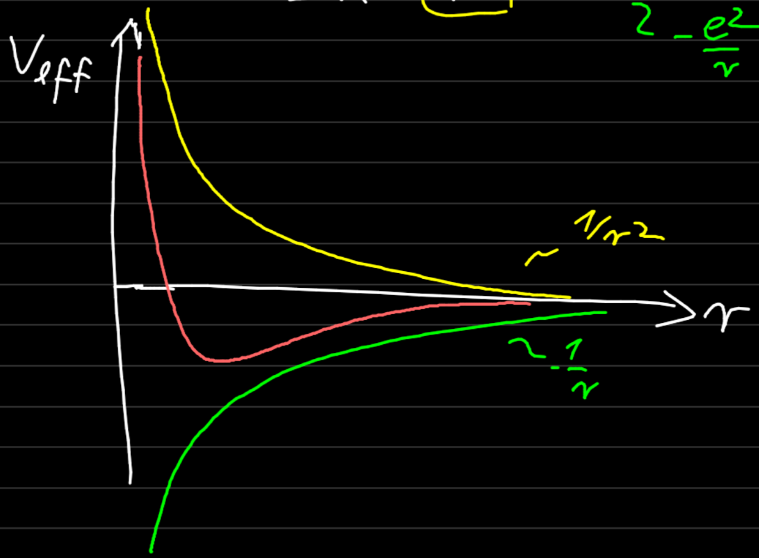
$$\rightarrow \boxed{E u(r) = \left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2 l(l+1)}{2M}\frac{1}{r^2} + V(r)\right) u(r)}$$

radiale Schröding. gl.

$\triangleq$ stat. Sch. gl. eines <u>1D</u>-Teilchens im eff. Potenzial

$$V_{eff}(r) = \frac{\hbar^2 l(l+1)}{2M}\boxed{\frac{1}{r^2}} + V(r)$$

$\sim -\frac{e^2}{r}$



Normierungs- und Randbed.:

$$\hookrightarrow 1 = \int_0^\infty dr\, r^2 \int_0^\pi d\vartheta \int_0^{2\pi} \sin\vartheta\, d\varphi \frac{|u|^2}{r^2} |Y_{l,m}|^2$$

$$= \int_0^\infty dr\, |u|^2$$

für $r \to \infty$ $\quad u(r) \leq \frac{1}{r^{1/2+\varepsilon}}$ ✓

$\varepsilon > 0$

$\underline{r \to 0}$: $\boxed{u(0) = 0}$

- $l \neq 0$: Stetigkeit von u
- $l = 0$: $\psi(r) = \frac{u(r)}{r}$

$\Rightarrow \Delta\psi = u(0)\,\underbrace{\Delta \frac{1}{r}}_{= 4\pi\,\delta(r)} = u(0)\,\cancel{\delta(r)}$

$r \to 0$

Verhalten für $u(r)$: $\boxed{r \to 0}$.

$$0 = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2}{2m} l(l+1)\frac{1}{r^2}\right) u(r) + \cancel{(V(r) - E)\,u(r)}$$

$|V(r)| \ll \frac{1}{r^2}$

$$u''(r) = l(l+1)\frac{u(r)}{r^2} \qquad r \to 0$$

$\to \boxed{u(r) = \alpha\, r^{l+1}} + \cancel{\beta r^{-l}}$

für $r \to 0$!

Verhalten für $r \to \infty$: $\quad V(r\to\infty) = 0$

gebundene Zust.: $\quad 0 > E = -|E|$

$$\to -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}u = -|E|\,u \cancel{- \left(\frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r)\right)}$$

$$u'' = \underbrace{\frac{2\mu|E|}{\hbar^2}}\, u \iff \boxed{u'' = q^2 u}$$

$$\Rightarrow q := \frac{\sqrt{2\mu|E|}}{\hbar}$$

$$\to \boxed{u(r) = \alpha e^{-qr}} + \cancel{\beta e^{+qr}}$$

→ Ansatz:

$$u(r) = r^{\ell+1} e^{-qr}\left(\alpha_0 + \alpha_1 r + \alpha_2 r^2 + \dots\right)$$

zweckmäßig:

substituieren $r \to x = qr$

$$\Rightarrow r = x/q$$

$$\frac{\partial}{\partial r} = \frac{\partial x}{\partial r}\frac{\partial}{\partial x} = q\frac{\partial}{\partial x}$$

rad. S gl.

$$0 = \left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2\ell(\ell+1)}{2\mu}\frac{1}{r^2} + V(r) + |E|\right)u$$

$$\Big\downarrow\; x = g r$$

$$0 = \left(\underbrace{-\frac{\hbar^2}{2\mu}\cdot g^2}_{-|E|}\frac{\partial^2}{\partial x^2} + \underbrace{\frac{\hbar^2\ell(\ell+1)}{2\mu}g^2}_{\ell(\ell+1)|E|}\cdot\frac{1}{x^2} + V(x/g) + |E|\right)u(x)$$

$$\rightarrow \boxed{0 = \left(-\frac{\partial^2}{\partial x^2} + \frac{\ell(\ell+1)}{x^2} + \frac{V(x/g)}{|E|} + 1\right)u(x)}$$

Wasserstoffatom

• e^-

• p

e^+

$m_p \gg m_e$

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

$$\frac{V(x/q)}{|E|} = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{|E|}\underbrace{q}_{=\sqrt{2m_e|E|}/\hbar}\cdot\frac{1}{x}$$

$$= -\boxed{\underbrace{\frac{\sqrt{2m_e}\,e^2}{4\pi\varepsilon_0\sqrt{|E|}\,\hbar}}_{=:x_0}}\cdot\frac{1}{x} = -\frac{x_0}{x}$$

$$\Rightarrow: \quad 0 = \left(\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} + \frac{x_0}{x} - 1\right)u(x) \quad *$$

Ansatz:

$$u(x) := x^{\ell+1} e^{-x}\, v(x)$$

in $(*)$ $\rightarrow$:

$$\boxed{x v'' + 2(\ell+1-x)v' + (x_0 - 2(\ell+1))v \overset{!}{=} 0} \quad (*)$$

$\hookrightarrow$ Lsg durch Potenzreihenansatz:

$$\boxed{v(x) = \sum_{\nu=0}^{\infty} a_\nu x^\nu}$$

(*)

$$0 = \sum_{\nu=0}^{\infty} a_\nu \Big\{ \nu(\nu-1)\, x^{\nu-1} + 2(\ell+1)\,\nu\, x^{\nu-1} - 2\nu\, x^{\nu} + (x_0 - 2(\ell+1))\, x^{\nu} \Big\}$$

$$= \sum_{\nu=0}^{\infty} \underbrace{\Big\{ a_{\nu+1}\big((\nu+1)\nu + 2(\ell+1)(\nu+1)\big) + a_\nu\big(x_0 - 2(\ell+1+\nu)\big) \Big\}}_{=0\,!}\, x^{\nu}$$

→ Rekursionsrelation:

$$a_{\nu+1} = \frac{2(\ell+1+\nu) - x_0}{\nu(\nu+1) + 2(\ell+1)(\nu+1)} \cdot a_\nu$$

Asymptotik: $\nu \gg 1$:

$$a_{\nu+1} \simeq \frac{2}{\nu} \cdot a_\nu$$

$$\to\; v(x) \simeq \sum_{\nu=0}^{\infty} \frac{(2x)^{\nu}}{\nu!} = e^{+2x}\ !$$

konvergente Lsgen falls Reihe abbricht bei $\nu = N$:

d.h. : $\underbrace{2(\ell+1+N)}_{\overset{!!}{n}} \overset{!}{=} x_0 = \frac{\sqrt{2m_e}\, e^2}{4\pi\varepsilon_0\, \hbar} \frac{1}{\sqrt{|E|}}$

Hauptquantenzahl

$$\Rightarrow \boxed{E_n = -\underbrace{\frac{m_e e^4}{(4\pi\varepsilon_0)^2 \hbar^2 \cdot 2}}_{E_{Ryd} \simeq 13{,}6\,eV} \frac{1}{n^2}} \quad n = 1, 2, 3, \ldots$$

Zustand: · Hauptq.z. n

· Drehimpulsq.z.

$\ell = 0, 1, \ldots, n-1$

· $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$

$\rightarrow E_n = -E_{Ryd} \cdot \frac{1}{n}$

Entartungsgrad: $\sum_{\nu=0}^{n-1} (2\nu+1) = D_n$

$$D_n = 2\underbrace{\sum_{\nu=0}^{n-1} \nu}_{= \frac{1}{2}(n-1)\cdot n} + n = \underline{\underline{n^2}}$$

n	ℓ		m	D_n
1 :	0	"s^1"	0	1
2 :	0	"s^2"	0	4
	1	"p^2"	$-1, 0, 1$	
3 :	0 :	"s^3"	0	9
	1 :	"p^3"	$-1, 0, 1$	
	2 :	"d^3"	$-2, -1, 0, +1, 2$	

$\underline{\underline{1/r}}$!

SO_3