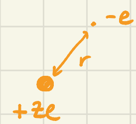
$1\ \text{esu} = \sqrt{1\ \text{dyn cm}^2}$

Review: SI and cgs units

Coulomb law $\quad \overset{\text{dyn}}{|\vec{F}|} = k_E \dfrac{q_1 q_2}{|\vec{r}|^2}, \qquad V = k_E \dfrac{q_1 q_2}{|\vec{r}|}$

SI units: $\quad k_E = \dfrac{1}{4\pi\varepsilon_0}$

cgs units: $\quad k_E = 1$



We will use cgs units for H atom (H-like atoms)

$$\Rightarrow \quad V = -\frac{Ze^2}{|\vec{r}|} = -\frac{Z\hbar c\alpha}{|\vec{r}|}$$

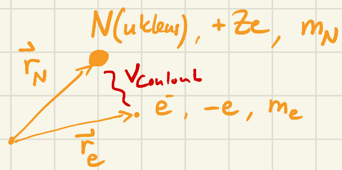
with dimensionless interaction strength $\alpha = \dfrac{e^2}{\hbar c} \simeq \dfrac{1}{137}$

$[\hbar c] = \text{Energie} \cdot \text{Länge} \qquad \left[\dfrac{\hbar c}{r}\right] = \text{Energie}$

9. Wasserstoffatom

$Z = 1$: Wasserstoffatom

$Z > 1$: H-ähnliche Atome



Hamiltonoperator: $\quad \hat{H} = \dfrac{\hat{\vec{p}}_N^{\,2}}{2m_N} + \dfrac{\hat{\vec{p}}_e^{\,2}}{2m_e} \underbrace{- \dfrac{Z\hbar c\alpha}{|\vec{r}_N - \vec{r}_e|}}_{\text{WW hängt nur von Relativkoord. ab}}$

→ **Schwerpunktsystem:**

Schwerpunktkoordinate: $\quad \vec{R}_{cm} = \dfrac{m_N \vec{r}_N + m_e \vec{r}_e}{m_N + m_e} \xrightarrow[m_N \gg m_e]{} \vec{r}_N$

$m_N \approx 2000\, m_e$

Relativkoordinate: $\quad \vec{r}_{rel} = \vec{r}_N - \vec{r}_e$

cm = center of mass

Zugehörigen Impulse

Schwerpunktimpuls: $\vec{P}_{cm} = \vec{P}_N + \vec{P}_e \xrightarrow{QM} \hat{\vec{P}}_{cm} = \frac{\hbar}{i} \frac{\partial}{\partial \vec{R}_{cm}}$

Relativimpuls: $\vec{P}_{rel} = \frac{m_e \vec{P}_N - m_N \vec{P}_e}{m_N + m_e} \xrightarrow{QM} \hat{\vec{P}}_{rel} = \frac{\hbar}{i} \frac{\partial}{\partial \vec{r}_{rel}}$

reduzierte Masse $m_r = \frac{m_N \cdot m_e}{m_N + m_e}$, Gesamtmasse $M = m_N + m_e$

$m_N \gg m_e$: $m_r \downarrow m_e$ $\qquad$ $m_N \gg m_e$: $M \downarrow m_N$

$$\hat{H} = \frac{\hat{\vec{P}}_N^2}{2m_N} + \frac{\hat{\vec{P}}_e^2}{2m_e} - \frac{Z\hbar c\alpha}{|\vec{r}_{rel}|}$$

$$\hat{H} = \frac{\hat{\vec{P}}_{cm}^2}{2M} + \frac{\hat{\vec{P}}_{rel}^2}{2m_r} - \frac{Z\hbar c\alpha}{|\vec{r}_{rel}|} = \hat{T}_{cm} + \hat{H}_{rel}$$

$$\Rightarrow \quad |\Psi\rangle = |\phi\rangle_{cm} |\psi\rangle_{rel} = |\vec{P}\rangle_{cm} |\psi_{rel}\rangle$$

$$\Psi(\vec{R}, \vec{r}) = \langle \vec{R}, \vec{r} | \Psi \rangle = \langle \vec{R} | \vec{P} \rangle \langle \vec{r} | \psi \rangle$$

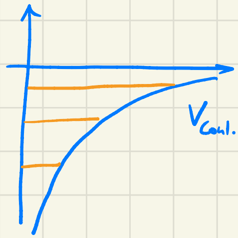
$$= e^{i \vec{P} \cdot \vec{R}} \quad \psi(\vec{r})$$

$\uparrow$ Wf für N-e⁻ Relativbew.

<u>Schrödingergleichung für Relativsystem</u> (rel weggelassen)

$$\left(\frac{\hat{\vec{P}}^2}{2m_r} - \frac{Z\alpha\hbar c}{|\vec{r}|} \right) \psi(\vec{r}) = E\, \psi(\vec{r})$$

Ziel: Lösung für gebundene e^-, $E<0$



Sphärisch sym. Pot.

$$\Rightarrow \quad \Psi(\vec{r}) = \frac{u_{E,\ell}(r)}{r} Y_\ell^m(\theta,\varphi) \quad \text{mit } u_{E,\ell}(r=0)=0$$

$$\Rightarrow \left(-\frac{\hbar^2}{2m_r}\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)\hbar^2}{2m_r r^2} - \frac{Z\alpha\hbar c}{r}\right) u_{E,\ell}(r) = E\, u_{E,\ell}(r)$$

↪ radiale S-Glg. für H-Atom

Gebundene Zustände mit $E = -\frac{\hbar^2}{2m_r}\kappa^2 < 0$, $\kappa = \sqrt{-2m_r E}$

Betrachte asymptotisches Verhalten für $u_{E,\ell}$ für $E<0$

$r \to 0$: dominiert $\frac{1}{r^2}$ vgl. zu $\frac{1}{r}$ (r-Verhalten wie freies Teilchen)

$$u_{E,\ell}(r) \sim r\, j_\ell(\ldots r) \sim r^{\ell+1}$$

$r \to \infty$: $\frac{1}{r^2}, \frac{1}{r}$ Terme $\to 0$ $\qquad u''_{E,\ell} = \kappa^2 u_{E,\ell} \qquad u_{E\ell}(r) \sim e^{-\kappa r}$

Betrachte dimensionslose Variable $\quad \rho = 2\kappa r$, $\rho_0 = 2\kappa r_0$

Typische Längenskala r_0 $\qquad |T| \sim |V| \qquad \frac{\hbar^2}{m_r}\frac{1}{r_0^2} = \frac{\hbar c\alpha}{r_0}$

$$\Rightarrow r_0 = \frac{\hbar}{m_r c\alpha} = \frac{\hbar c}{m_r c^2 \alpha} = \frac{\hbar^2}{m_r e^2} \qquad \text{Bohr radius}$$

Definiere: $\nu \equiv \dfrac{Z}{\varkappa r_0}$ $\longrightarrow$ Energie

Radiale S-Ggl. in dim. Variablen ρ

$$\boxed{\left(\frac{\partial^2}{\partial \rho^2} - \frac{\ell(\ell+1)}{\rho^2} + \frac{\nu}{\rho} - \frac{1}{4} \right) u_{E\ell}(\rho) = 0} \qquad \circledast$$

Ansatz: $u_{E,\ell}(\rho) = \rho^{\ell+1} e^{-\rho/2} \, \tilde{u}_{E\ell}(\rho) \cdot \mathcal{N}$

mit Potenzreihenansatz für $\tilde{u}_{E\ell}(\rho) = \sum\limits_{n=0}^{\dots} c_n \rho^n$

$\longrightarrow$ werden sehen, dass Reihe endlich sein muss

Ansatz einsetzen in $\circledast$: DGL für $\tilde{u}_{E,\ell}$

$$\Rightarrow \quad \rho \, \tilde{u}_{E\ell}'' + (2\ell+2-\rho) \, \tilde{u}_{E\ell}' - (\ell+1-\nu) \, \tilde{u}_E = 0 \qquad \circledast\circledast$$

Potenzreihe einsetzen:

$$\cancel{\rho} \sum_{\substack{n=2 \\ \cancel{n=1} \\ n=0}} \underset{n+1}{c_n} \; \underset{n+1}{n} \underset{n}{(n-1)} \; \underset{\rho^n}{\rho^{n-\cancel{2}\,1}} + (2\ell+2-\rho) \sum_{\substack{n=1 \\ n=0}} \underset{n+1}{c_n} \cdot \underset{n+1}{n} \, \underset{n}{\rho^{n-1}} - (\ell+1-\nu) \sum_{n=0} c_n \rho^n = 0$$

$$\Leftrightarrow \quad \sum_{n=0} \rho^n \left[-(\ell+1-\nu) c_n - c_n n + (2\ell+2) \, c_{n+1} (n+1) + c_{n+1} (n+1) \cdot n \right] = 0$$

$\Rightarrow$ jeder Koeff $[\dots] = 0 \quad \forall n$

$$\Rightarrow \quad c_{n+1}\left(n(n+1) + (2\ell+2)(n+1)\right) - c_n\left(\ell+1-\nu+n\right) = 0$$

$$\Rightarrow \quad c_{n+1} = \frac{\ell+1-\nu+n}{(n+1)(2\ell+2+n)}\, c_n$$

Starte mit $c_0 = 1$, Normierung von $\tilde{u}_{E,\ell}$ am Ende

$$\Rightarrow \quad c_n = \frac{1}{n!}\,\frac{\Gamma(2\ell+2)}{\Gamma(2\ell+2+n)}\,\frac{\Gamma(\ell+1-\nu+n)}{\Gamma(\ell+1-\nu)}$$

$\nu = \frac{Z}{\varkappa r_0}$

$\varkappa = \sqrt{-2m_e E}$

mit Gammafkt. $\Gamma(n+1) = n! \quad n \in \mathbb{N}$

$$\Gamma(x+1) = x\,\Gamma(x)$$

$$\Rightarrow \quad \tilde{u}_{E,\ell}(\rho) = \sum_{n=0} \frac{(2\ell+1)!}{(2\ell+1+n)!}\,\frac{\Gamma(\ell+1-\nu+n)}{\Gamma(\ell+1-\nu)}\,\frac{\rho^n}{n!}$$

$$= {}_1F_1\left(\ell+1-\nu,\, 2\ell+2,\, \rho\right)$$ falls Reihe unendl.

Konfluente hypergeometrische Fkt.

$${}_1F_1(a,\alpha,\rho) = \sum_{n=0}^{\infty} c_n \rho^n, \quad c_0 = 1$$

$$c_{n+1} = \frac{1}{(n+1)!}\,\frac{a(a+1)\cdots(a+n)}{\alpha(\alpha+1)\cdots(\alpha+n)}$$

$$\xrightarrow{\text{unendl. Reihe}} \rho^{a-\alpha}\, e^{\rho} \quad \text{für } \rho \to \infty$$

$$\rho^{-\ell-1-\nu}\, e^{\rho}$$ zerstört Normierbarkeit!

$\Rightarrow$ Potenzreihe <u>muss</u> abbrechen

$\Rightarrow \boxed{a = -k}$, $k = 0, 1, 2, \ldots$, $l = 0, 1, 2, \ldots$

$\Rightarrow l + 1 - \nu = -k$ Energiequantisierung

$$\boxed{n \equiv \nu = l + 1 + k} \qquad \boxed{n = 1, 2, 3, \ldots}$$

$\uparrow$ Hauptquantenzahl

$\nu = \frac{Z}{\kappa r_0}$

$r_0 = \frac{\hbar}{m_r c \alpha} = \frac{\hbar^2}{m_r e^2}$

$$\Rightarrow \kappa = \frac{m_r c \alpha Z}{\hbar n} = \frac{m_r c^2 \alpha Z}{\hbar c \cdot n} = \frac{m_r e^2 Z}{\hbar^2 \cdot n}$$

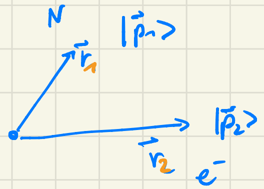
$\frac{1}{r_0}$

$$\boxed{E} = -\frac{\hbar^2 \kappa^2}{2 m_r} = -\frac{m_r c^2 \alpha^2 Z^2}{2} \frac{1}{n^2} = -\frac{m_r e^4 Z^2}{2\hbar^2} \frac{1}{n^2} = \boxed{-\frac{R_y Z^2}{n^2}}$$

Rydbergzahl $\quad R_y = \frac{m_r c^2 \alpha^2}{2} = \frac{m_r e^4}{2\hbar^2}$

$$\approx \frac{m_e c^2 \alpha^2}{2} = \frac{511\,\text{keV} \left(\frac{1}{137}\right)^2}{2} = 13{,}6\,\text{eV}$$

Grundzustand $n = 1$: $E_1 = -13{,}6\,\text{eV}\, Z^2 \underset{\text{H-Atom}}{=} -13{,}6\,\text{eV}$



ohne $V_{Coul.}$

$$|\Psi\rangle = |\vec{p}_1\rangle_1 \otimes |\vec{p}_2\rangle_2$$

$$\langle \vec{r}_1, \vec{r}_2 | \Psi \rangle = \langle \vec{r}_1 | \vec{p}_1 \rangle \langle \vec{r}_2 | \vec{p}_2 \rangle = \psi_{\vec{p}_1}(\vec{r}_1)\, \psi_{\vec{p}_2}(\vec{r}_2)$$