QMI-5 bodová částice ve 3D-centrální potenciálové pole

OPAKOVÁNÍ: $H,\ L^2,\ L_z$ $\qquad \psi_{klm}(x,y,z) = R_{kl}(r)\,Y_{lm}(\theta,\varphi)$

5a) $\hat{H} = \hat{T} + V(\vec{x})$ $\qquad V(\vec{x}) = r = |\vec{x}|$

V .. po částech konst. fce

$j_e, m_e, k_e^{(\pm)}$

cvičení

5b) Částice v Coulombickém poli

$V(r) = \frac{\gamma}{r}$ $\qquad \gamma < 0 \quad -|\gamma|$

motivace: → atom vodíku

→ 1ele. ionty Li^{++} .. př.

→ μ^--H atom ; pozitronium e^+-e^- , $\bar{p}$-p protonium

$\bar{H}$

• idealizace .. centrum $m \to \infty$ (BÚNO) .. CMS

• symetrie Rungelenzův vektor $\vec{A} = \vec{p} \times \vec{L} - m\gamma \frac{\vec{r}}{|\vec{r}|}$

$= m\gamma\,\vec{e}$.

$\forall$ centrální pole .. $\vec{L}$

$\forall$ syst. $\frac{\partial}{\partial t}A$ ... E

→ $\hat{H}|\psi\rangle = E|\psi\rangle$ .. separuje v sférických souř.

ale i v

→ parabolických, eliptických

$R(r)$

$r\,\chi_{El}(r)\,Y_{lm}(\theta,\varphi)$

$\boxed{\text{Řešení tj. nalezení } |E, l m\rangle \;..\; \psi_{Elm}(\vec{x})}$

$$\chi''(r) + \underbrace{\frac{2m}{\hbar^2}}\left(E + \frac{|\gamma|}{r} - \frac{\hbar^2 l(l+1)}{2mr^2}\right)\chi(r) = 0$$

$\rho = \beta r \;..\; \beta = 1/\text{délka} \;...\; \underline{\chi(r) = u(\rho)}$

$$u''(\rho) + \underbrace{\frac{2mE}{\hbar^2\beta^2}}_{\to -\frac{1}{4}} u + \boxed{\frac{2m|\gamma|}{\hbar^2\beta}}\frac{u}{\rho} - \frac{l(l+1)}{\rho^2}u = 0$$

volba beta

konvence

$$\boxed{\lambda = \frac{2m|\gamma|}{\beta\hbar^2}} = \frac{|\gamma|}{\hbar}\sqrt{\frac{m}{2|E|}}$$

$\beta = \frac{\sqrt{8m|E|}}{\hbar}$ — $E = -|E| < 0$ vázané stavy

$$u''(\rho) + \left[-\frac{1}{4} + \frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2}\right]u = 0 \qquad (*)$$

Řešení: regulární $\rho \to 0$ $u(\rho)\begin{cases}\boxed{\rho^{l+1}} \\ \cancel{\rho^{-l}}\end{cases}$

$u(\rho) = 0$ tj.

$\rho \to \infty$ $u'' = \frac{1}{4}u$ $u(\rho) = e^{-\rho/2}$

řešení $e^{+\rho/2}$ není z $L^2(\mathbb{R}^3)$

$$u(\rho) = \rho^{l+1} e^{-\rho/2} w(\rho), \;...\; e^{\rho} \longrightarrow \rho^{+}\rho/2$$

$\to$ dosazdo $(*)$.

$$\rho w'' + \underline{(2l+2-\rho)}\, w' + [\lambda - (l+1)]\, w = 0$$

ODBOČKA řešení ODR (ODE) $w'' + p(z)w' + q\, w = 0$

(.. Formánek

b^2) Gaussova rovnice $\quad / \tilde{b}$

$$\frac{z}{b}\left(1-\cancel{\frac{z}{b}}\right)\bar{w}'' + \left[c-(1+a+b)\frac{z}{b}\right]\bar{w}' - ab\,\bar{w} = 0$$

Hypergeometrická fce $\quad \bar{w} = c_0 + c_1 z + c_2 z^2 + \dots$

$$F(a,b,c,z) = 1 + \frac{ab}{c}\frac{z}{1!} + \frac{a(a+1)\,b(b+1)}{c(c+1)}\frac{z^2}{2!} + \dots$$

$$+ \frac{a(a+1)\dots(a+k-1)\,b(b+1)\dots(b+k-1)}{c(c+1)\dots(c+k-1)}\frac{z^k}{k!}\dots$$

Gaussova rce má 2 LNZ řešení:

$\bar{w}_1(\rho) = F(a,b,c,\rho)$

$\bar{w}_2(\rho) = \rho^{1-c}F(1+a-c,2-c,\rho)$ ... singulární v poč

Degenerovaná Gaussova rovnice

$$\rho w'' + (c-\rho)w' + a w = 0$$

$$F(a,c,\rho) = \lim_{b\to\infty} F\left(a,b,c,\frac{\rho}{b}\right)$$

$$w_1\ F(a,c,\rho) = 1 + \frac{1}{1!}\frac{a}{c}\rho + \frac{1}{2!}\frac{a(a+1)}{c(c+1)}\rho^2 + \dots$$

$$\cancel{w_2 = \rho^{1-c}F(1+a-c,2-c,\rho)}$$ ... singul. v poč

$$c = 2(l+1) \qquad \underbrace{a = l+1-\lambda} = -\nu$$

... analýza řady ... $F(\rho) \xrightarrow[\rho\to\infty]{} e^{\rho}$

→ jen konečný počet členů

$a \quad a+1 \quad \ldots \quad a+k$

pro $a = 0, -1, -2 \ldots$ se řada redukuje na polynom

$a = -\nu$ kde $\nu \in \mathbb{Z}_0^+$

$a = -\nu = l+1-\lambda$

$\lambda = l+1+\nu = n$

$\lambda^2 = \frac{\gamma^2}{\hbar^2} \frac{m}{2|E|}$

$E_n = -\frac{m\gamma^2}{2\hbar^2 (l+1+\nu)^2}$

$\boxed{E_n = -\frac{R}{n^2}}$ hlavní kvant. číslo

v případě atomu vodíku $\gamma = -\frac{e^2}{4\pi\varepsilon_0}$

$R = \frac{m(\gamma^2)}{2\hbar^2} = R_y$ Rydbergova konst. $= 13{,}6\,\mathrm{eV}$

$n = \overset{0}{l} + 1 + \overset{0}{\nu}$ $\quad 0, 1, 2, \ldots$

$n = 1, 2, 3, \ldots \in \mathbb{N}$ –

$l = 0, 1, \ldots, n-1 \quad \ldots \quad n$

$m = -l, -l+1, \ldots l \quad \ldots \quad 2l+1$ hodnot.

$E_n \ldots \quad R_{nl} = \beta r\, (\beta r)^{l+1} e^{-(\beta r)/2} F(\qquad)$

$Y_{lm} \quad 2l+1$

$\rightarrow N = \sum_{l=0}^{n-1} (2l+1) = n^2$

$\forall E_n \ldots n^2 \times$ degenerovaná

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konstanty .. $Ry = 13.6\,eV$ .. $E_n = -\frac{Ry}{n^2}$

(atom vodíku) $\boxed{\gamma = -\frac{e_0^2}{4\pi\varepsilon_0}}$

$$\rho = \beta r = \frac{\sqrt{2m|E_n|}}{\hbar} r = \frac{\sqrt{4m\frac{m\gamma^2}{\hbar^2 n^2}}}{\hbar} = \frac{2m|\gamma|}{\hbar^2 n} r$$

$$\frac{\hbar^2}{m|\gamma|} = a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e_0^2}$$ Bohrův poloměr atomu vodíku

$$= 0{,}53\,Å = 0.53\cdot 10^{-10}\,m$$

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vlnové funkce:

$$R_{nl}(r) = N_{nl}\Big(\underbrace{\frac{2r}{na_0}}_{\rho}\Big)^l \underbrace{F(-\nu, 2(l+1), \rho)}_{\text{(zobecněné) Laguerrovy polynomy}} e^{-\rho/2}$$

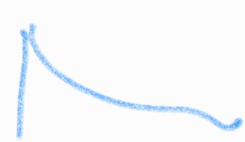
$l=0$

$$L_n^\alpha(x) \equiv \binom{n+\alpha}{n} F(-n, \alpha+1, x)$$

$$\to R_{nl}(r) = \frac{2}{n}\sqrt{\frac{(n-l-1)!}{(n+1)!}}\, a^{-3/2}\left(\frac{2r}{na}\right)^l L_\nu^{2l+1}\left(\frac{2r}{na}\right) e^{-\frac{r}{na}}$$

- $$L_n^\alpha(x) = \underbrace{\sum_{m=0}^{n} (-1)^m \binom{n+\alpha}{n-m}\frac{x^m}{m!}}_{\text{řada } F} = \underbrace{\frac{1}{n!}e^x x^{-\alpha}\frac{d^n}{dx^n}\left(e^{-x}x^{n+\alpha}\right)}_{\text{algebraický}}$$
- ortogonální polynomy $1, x, x^2, x^3, \ldots$ G-S ob

$$\int_0^\infty L_n^\alpha(x)\, L_{n'}^\alpha(x)\, x^\alpha e^{-x}\, dx$$



$R_{10}(r) = 2\sqrt{\frac{1}{a^3}}\, e^{-r/a}$ .. základní stav $n=1$, $l=0$, $m=0$

1. excitovaný stav: $n=2$ ... $\underline{l=0}$ $m=0$

$\underline{l=1}$ $m=0,\pm1$

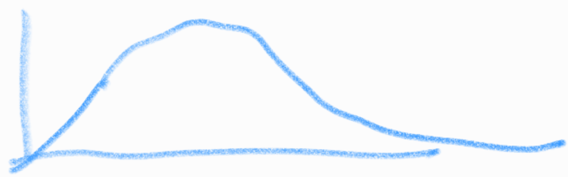
$$R_{20}(r)=\underbrace{\sqrt{\frac{1}{2a^3}}\left[1-\frac{r}{2a}\right]}e^{-r/2a} \qquad 1 \quad L^1 \quad \nu=1$$

$$R_{21}(r)=\frac{1}{2}\underbrace{\sqrt{\frac{1}{6a^3}}\,\frac{r}{a}}e^{-r/2a} \quad \dots \quad 0 \quad L^3 \quad \nu=0$$

počet kořenů

$\nu = n-l-1$

r^l



$n,\ {}^{l}_{m}$

5c Izotropní harmonický oscilátor

$$V(r)=\frac{1}{2}m\omega^2\underbrace{(x^2+y^2+z^2)}_{r^2} \quad \dots \quad \mathcal{H}=\mathcal{H}_x\otimes\mathcal{H}_y\otimes\mathcal{H}_z$$

$\{H_x, H_y, H_z\}$ ÚSKO 1D LHO $\phi_n(x)$

$$\hookrightarrow \hat{H} \ \dots \ E_{n_xn_yn_z}=E_{n_x}+E_{n_y}+E_{n_z}=\hbar\omega\left(\frac{3}{2}+N\right)$$

$N=n_x+n_y+n_z$ $\quad 0+5+0=1+3+1$

$$\langle\vec{x}|n_xn_yn_z\rangle \quad \phi_{n_xn_yn_z}(\vec{x})=\phi_{n_x}(x)\,\phi_{n_y}(y)\,\phi_{n_z}(z)$$

$\|$

$|n_x\rangle\otimes|n_y\rangle\otimes|n_z\rangle$ kartézské řešení sférické řešení: $\{\hat{H}, L^2, L_z\}$ ... $V(r)$

$\mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_{S_2}$

$$\psi_{Elm}(x) = R_{nl}(r)\, Y_{lm}(\theta,\varphi) \qquad \chi = rR$$

$$\chi''(r) + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2 r^2 - \frac{\hbar^2 l(l+1)}{2mr^2}\right)\chi = 0$$

$$x_0 = \sqrt{\frac{\hbar}{m\omega}} \qquad r = \rho x_0 \qquad \chi(r) = u(\rho)$$

$$u'' + \Big(\underbrace{\frac{2E}{\hbar\omega}}_{\lambda} - \underbrace{\rho^2} - \cancel{\frac{l(l+1)}{\rho^2}}\Big)u = 0$$

asymtotika: $\rho \to 0$ ... $u \sim \rho^{l+1}$ $\cancel{\rho^{-l}}$

$\rho \to \infty$ $\quad u'' - \rho^2 u = 0 \qquad e^{-\frac{1}{2}\rho^2}$

$$u(\rho) = \rho^{l+1} e^{-\frac{1}{2}\rho^2} w(\rho)$$

$$\Rightarrow w'' + \frac{2}{\rho}\left((l+1) - \rho^2\right)w'(\rho) + (\lambda - 2l - 3)w = 0$$

$\rightarrow \quad z = \rho^2 \qquad w(\rho) = v(z)$

$$z v'' + (\underbrace{l + \tfrac{3}{2}}_{c} - z)v' + \underbrace{\left(\frac{\lambda}{4} - \frac{l}{2} - \frac{3}{4}\right)}_{-a} v = 0$$

... $F(a, c, z)$ ... $z \to \infty$ $\quad e^z$ $\qquad \nu = 0, 1, 2, \ldots$

$\rightarrow$ redukce na polynom ... $a = -\nu$

$$\frac{3}{4} + \frac{l}{2} - \frac{\lambda}{4} = a = -\nu \qquad l = 0, 1, 2, \ldots$$

$$E = 4 \cdot \frac{\hbar\omega}{2}\left(\nu + \frac{l}{2} + \frac{3}{4}\right) = \hbar\omega\left(\frac{3}{2} + \boxed{2\nu + l}\right)$$

degenerace ? E_N kart. $\quad E_\Lambda$ sférické

$\Lambda = 2\nu + l \qquad m = -l \dots l$

Λ sudé ... $l = 0, 2, \dots \Lambda \quad N_{deg} = \sum_{l=0,2}^{\Lambda} (2l+1) = \frac{(\Lambda+1)(\Lambda+2)}{2}$

Λ liché ... $l = 1, 3, \dots \Lambda \quad N_{deg} = \sum_{l=1,3}^{\Lambda} (2l+1) = \frac{1}{2}\left(\frac{\Lambda+1}{2}\right)(2\Lambda+4)$

$$N_{deg} = \frac{(\Lambda+1)(\Lambda+2)}{2}$$

kartézské ... $N = n_x + n_y + n_z$

$n_x \quad n_y \quad n_z$

$n_y = 0$

$N+1$

$$\frac{(N+1)(N+2)}{2}$$

Gauss: $\quad z(1-z)w'' + [c - (1+a+b)z]w' - abw = 0 \qquad (6)$

Hyperg. fce $\quad F(a,b,c,z) = 1 + \frac{ab}{c}\frac{\varrho}{1!} + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{\varrho}{2!} + \dots$

Degenerovaná Gauss rovnice

Degener. Hyperg. fce $\quad F(a,c,\varrho) = \lim_{b\to\infty} (a,b,c,\frac{\varrho}{b}) = w(\varrho)$

$(6) \to \quad z = \frac{\varrho}{b} \qquad \boxed{b \to \infty} \qquad \frac{dw}{dz} = b\frac{dw}{d\varrho}$

$dz = \frac{d\varrho}{b}$

$$\frac{\cancel{\rho}}{\cancel{b}}\left(1-\cancel{\frac{\rho}{b}}\right)\cancel{b^2}\, w'' + \Big[c - (\underbrace{1+a}_{\to 1}+\cancel{b})\frac{\rho}{\cancel{b}}\Big]\cancel{b}\, w' - a\cancel{b}\, w = 0$$

$$\rho\, w'' + [c-\rho]\, w' - a\, w = 0$$

$$\frac{a(a+1)\cdots(a+k-1)\, b(b+1)\cdots(b+k-1)}{c(c+1)\cdots(c+k-1)}\, \frac{\rho^k}{k!\, b^k}$$

$$\xrightarrow[b\to\infty]{} 1 \qquad\qquad \frac{b+n}{b} \to 1$$