L9

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Radial Wave Functions of Hydrogen-Like Atoms

$R_{nl}(r) = \frac{u(r)}{r}$; $a = \frac{\hbar}{mc\alpha}$

$E_n = -\frac{Z^2\alpha^2 mc^2}{2n^2}$

$e^2 = \alpha\hbar c$

$\rho = \frac{Z\cdot r}{n\cdot a}$

$$\frac{d^2u}{d\rho^2} + \left(-1 - \frac{\ell(\ell+1)}{\rho^2} + \frac{2n}{\rho}\right)u(\rho) = 0$$

- we know $R_{n\ell}(r)\big|_{r\to 0} \sim r^{\ell}$, $u(r)\big|_{r\to 0} \sim \rho^{\ell+1}$

Define $u(\rho) = \rho^{\ell+1} g(\rho)$ $\Leftarrow$ $g(\rho)\big|_{\rho\to 0} \to \text{const}$

$u'(\rho) = (\ell+1)\rho^{\ell} g(\rho) + \rho^{\ell+1} g'(\rho)$

$u''(\rho) = \ell(\ell+1)\rho^{\ell-1} g(\rho) + (\ell+1)\rho^{\ell} g'(\rho) + (\ell+1)\rho^{\ell} g'(\rho) + \rho^{\ell+1} g''(\rho)$

HW

$$g''(\rho) + \frac{2(\ell+1)}{\rho} g'(\rho) + \left(\frac{2n}{\rho} - 1\right) g(\rho) = 0$$

define $g(\rho) = e^{-\rho} f(\rho)$

$g'(\rho) = -e^{-\rho} f(\rho) + e^{-\rho} f'(\rho)$

$g''(\rho) = e^{-\rho} f(\rho) - e^{-\rho} f'(\rho) - e^{-\rho} f'(\rho) + e^{-\rho} f''(\rho)$

$$\rho f''(\rho) + 2(\ell+1-\rho) f'(\rho) + 2(n-\ell-1) f(\rho) = 0$$

what if $m_{max} = \infty$

searching $f(\rho) = \sum_{m=0}^{m_{max}} a_m \rho^m$ a_0

$(a_0 + a_1\rho^1 + a_2\rho^2 + \dots)'$

$f'(\rho) = \sum_{m=1}^{m_{max}} m a_m \rho^{m-1}$ ~~$m=1$ a_1~~

$f''(\rho) = \sum_{m=2}^{m_{max}} m(m-1) a_m \rho^{m-2}$

$$\sum_{m=2}^{m_{max}} m(m-1) a_m \rho^{m-1} + 2(\ell+1-\rho)\sum_{m=1}^{m_{max}} m a_m \rho^{m-1} + 2(n-\ell-1)\sum_{m=0}^{m_{max}} a_m \rho^m = 0$$

$m = \tilde{m}+1$

$m = \tilde{m}+2$

$$\sum_{m=0}^{m_{max}-2} (m+2)(m+1) a_{m+2}\rho^{m+1} + 2(\ell+1-\rho)\sum_{m=0}^{m_{max}-1} (m+1) a_{m+1}\rho^m + 2(n-\ell-1)\sum_{m=0}^{m_{max}} a_m \rho^m = 0$$

ρ^m $\rho^{m_{max}}$

(a) $\sum_{m=0}^{m_{max}-2} (m+2)(m+1) a_{m+2}\rho^{m+1} - 2\sum_{m=0}^{m_{max}-1} (m+1) a_{m+1}\rho^{m+1} +$

$\rho^{m_{max}-1}$ $\rho^{m_{max}}$

(b) maxful ρ power $\rho^{m_{max}-1}$ $+ 2(\ell+1)\sum_{m=0}^{m_{max}-1} (m+1) a_{m+1}\rho^m + 2(n-\ell-1)\sum_{m=0}^{m_{max}} a_m \rho^m = 0$

$\longrightarrow -2\, m_{max}\, a_{m_{max}}\rho^{m_{max}}$

$+$

$2(n-\ell-1)\, a_{m_{max}}\rho^{m_{max}} = 0$

$\Rightarrow$ lower Power of ρ is 0

$$2(\ell+1) a_1 \rho^0 + 2(n-\ell-1) a_0 \rho^0 = 0$$

$$a_1 = -\frac{n-\ell-1}{\ell+1} a_0$$

$\Rightarrow$ Identify m power of ρ $[\rho^m]$

$$(m+1)m\, a_{m+1}\rho^m - 2m\, a_m \rho^m + 2(\ell+1)(m+1) a_{m+1}\rho^m + 2(n-\ell-1) a_m \rho^m = 0$$

$$a_m\big(2(n-\ell-1-m)\big) + a_{m+1}\big[m(m+1) + 2(\ell+1)(m+1)\big] = 0$$

$2(n-\ell-1-m)$ $2(n-\ell-1-m)$

$$a_{m+1} = -\frac{2(m \ldots)}{(m+1)(m+2(\ell+1))} a_m = -\frac{2(m \ldots)}{(m+1)(m+2\ell+2)} a_m$$

Check $m=0$

$$a_1 = -\frac{2(n-\ell-1)}{2\ell+2} a_0 = -\frac{(n-\ell-1)}{\ell+1} a_0$$

$$\frac{a_{m+1}}{a_m} = \frac{-2(n-\ell-1 \ldots}{(m+1)(m+\ldots}$$

$m_{max} \to \infty$

$m \to \gg$ large

$m \gg$

$$\frac{a_{m+1}}{a_m} = \frac{+2m}{m^2}$$

$m >$

⇒ Calculating m_{max}

$$-2 m_{max} \cancel{a_{m_{max}}} \cancel{\rho^{m_{max}}} + 2(n-\ell-1) \cancel{a_{m_{max}}} \cancel{\rho^{m_{max}}} = 0$$

$$-2 m_{max} + 2(n-\ell-1) = 0$$

$$\boxed{m_{max} = n-\ell-1}$$

$\boxed{\ell \le n-1}$

$$f(\rho) = \sum_{m=0}^{m_{max}} a_m \rho^m = \sum_{m=0}^{n-\ell-1} a_m \rho^m$$

if $n-\ell-1 < 0$ there is no solution.

- Solution exists $\boxed{n-\ell-1 \ge 0}$

$$\boxed{\ell \le n-1}$$

- why m_{max} is finite

- if it is not finite

m_{max} can not be infinity

$$\frac{a_{m+1}}{a_m} = \frac{2}{m} \Big|_{m \to \infty}$$

$$f(\rho) = \sum_{m=0}^{\infty} a_m \rho^m \sim \cancel{e^{2\rho}} \Big|_{\rho \to \infty}$$

— no

- Lets take $e^{2\rho} = \boxed{\sum_m \frac{(2\rho)^m}{m!}} = \sum_m \frac{2^m}{m \ldots}$

term $\to a_m = \frac{2^m}{m!}$

$$\frac{a_{m+1}}{a_m} = \frac{2^{m+1}}{(m+1)!} \frac{m!}{2^m}$$

$a \ldots \; 2^{m+1}$

$$a_{m+1} = \frac{2}{(m+1)!}$$

⟹ Summarizing

$$R_{El}(r) = \frac{U(r)}{r}, \quad U(\rho) = \rho^{l+1} \cdot g(\rho)$$

$$g(\rho) = e^{-\rho} f(\rho)$$

$$f(\rho) = \sum_{m=0}^{n-l-1} a_m \rho^m$$

$$R_{El}(r) \equiv R_{nl}(r)$$

$$\boxed{\rho = \frac{Z \cdot r}{n \cdot a}, \quad a = \frac{\hbar}{mc\alpha}}$$

$$\boxed{R_{nl}(r) = \frac{\rho^{l+1} e^{-\rho} \sum_{m=0}^{n-l-1} a_m \rho^m}{r}}$$

⟹ Ground state of Hydrogen Atom

$\boxed{l \le n-1}$

$Z=1$, $\rho = \frac{r}{na}$

Ground state $n=1$, $l=0$;

$$R_{10}(r) = \frac{\rho e^{-\rho} \sum_{m=0}^{0} a_m \rho^m}{r} = \frac{\rho e^{-\rho} a_0}{r} = \frac{r}{a \cdot r} e^{-\frac{r}{a}} \cdot a_0$$

Bohr radius

$$R_{10}(r) = \frac{1}{a} e^{-\frac{r}{a}} \cdot a_0 \text{ — coefficient.}$$

$a_0 = ?$

$$\int |R_{10}(r)|^2 r^2 dr = 1$$

$$\frac{a_0^2}{a^2} \int_0^\infty e^{-\frac{2r}{a}} r^2 dr = 1$$

Solve $a_0 = ?$

Calculate

$$\int_0^\infty e^{-\frac{2r}{a}} r^2 dr = -\frac{a}{2} \int_0^\infty d e^{-\frac{2r}{a}} r^2 = -\frac{a}{2} e^{-\frac{2r}{a}} r^2 \Big|_0^\infty + \frac{a}{2} \int_0^\infty e^{-\frac{2r}{a}} 2r dr =$$

$$= a\int_0^\infty e^{-\frac{2r}{a}} r\,dr = -\frac{a^2}{2}\int_0^\infty d\left(e^{-\frac{2r}{a}}\right) r = -\frac{a^2}{2} e^{-\frac{2r}{a}} r\Big|_0^\infty + \frac{a^2}{2}\int_0^\infty e^{-\frac{2r}{a}}\,dr =$$

$$= -\frac{a^3}{4} e^{-\frac{2r}{a}}\Big|_0^\infty = \boxed{\frac{a^3}{4}}$$

$$\boxed{\frac{a_0^2}{a^2}\frac{a^3}{4} = 1} \qquad a_0^2 a = 4 \qquad \boxed{a_0 = \frac{2}{\sqrt{a}}}$$

Thus $\boxed{R_{10}(r) = \frac{2}{a^{3/2}} e^{-\frac{r}{a}}}$

Total Wave Function

$$\boxed{\Psi_{\substack{000\\ n\ell m}}(r,\theta,\varphi)} = R_{10}(r)\, Y_0^0(\theta,\varphi) = \frac{2}{a^{3/2}} e^{-\frac{r}{a}} \boxed{\frac{1}{\sqrt{4\pi}}} = \boxed{\frac{1}{\sqrt{a^3\pi}} e^{-\frac{r}{a}}}$$

$\Rightarrow$ Calculation for $n=2$ $\ell=0$

Remember $R_{n\ell}(\rho) = \frac{\rho^{\ell+1} e^{-\rho}}{r}\sum_{m=0}^{n-\ell-1} a_m\rho^m$ $\qquad \rho = \frac{Z\cdot r}{na}$

$$R_{20}(r) = \frac{\left(\frac{r}{2a}\right) e^{-\frac{r}{2a}}}{r}\sum_{m=0}^{1} a_m\rho^m = \frac{1}{2a} e^{-\frac{r}{2a}}\left(a_0 + a_1\rho^1\right)$$

$\rho = \frac{r}{2a}$

Remember: $\boxed{a_{m+1} = \frac{-2(n-\ell-1-m)}{(m+1)(m+2\ell+2)} a_m}$

$$a_1 = -\frac{2(2-1)}{2} a_0 \qquad a_1 = -a_0$$

$$R_{20}(r) = \frac{1}{2a} e^{-\frac{r}{2a}}\left(a_0 - a_0\frac{r}{2a}\right) = \frac{a_0}{2a}\left(1-\frac{r}{2a}\right) e^{-\frac{r}{2a}}$$

$2a$

na

$$\int_0^\infty |R_{20}(r)|^2 r^2\,dr = 1$$

R_{21} ($\ell=1$)