

Renew Bohr model

$$\alpha = \frac{ke^2}{\hbar c}$$

skip?

skip

me

$$F = F$$

$$\mu \frac{v^2}{r} = \frac{ke^2}{r^2} = \frac{\alpha \hbar c}{r}$$

$$v^2 = \frac{\alpha \hbar c}{\mu r}$$

$$L = \mu v r$$

$$L^2 = \mu^2 v^2 r^2 = \mu^2 r^2 \left(\frac{\alpha \hbar c}{\mu r} \right) = \alpha \mu \hbar c r$$

$$r = \frac{L^2}{\alpha \mu \hbar c}$$

$$\text{Bohr: } L = n \hbar \Rightarrow r = \frac{n^2 \hbar}{\alpha \mu c}$$

$$n=1 \Rightarrow a_0 = \frac{\hbar}{\alpha \mu c} \approx 0.529 \text{ \AA}$$

$$E = \frac{1}{2} \mu v^2 - \frac{ke^2}{r}$$

$$= -\frac{1}{2} \frac{ke^2}{r} = -\frac{1}{2} \frac{\alpha \hbar c}{r} = -\frac{1}{2} \alpha \hbar c \left(\frac{\alpha \mu c}{n^2 \hbar} \right)$$

$$= -\frac{1}{2} \frac{\alpha^2 \mu c^2}{n^2}$$

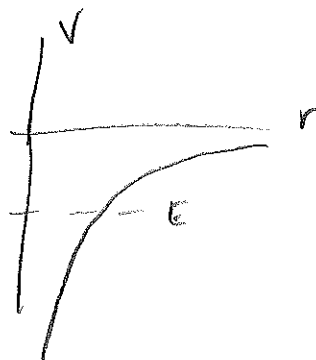
$$= -\frac{\left(\frac{1}{2} \alpha^2 \mu c^2 \right)}{n^2} = -\frac{(13.6 \text{ eV})}{n^2}$$

Hydrogen atom

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$$-\frac{\hbar^2}{2m} \nabla^2 u + V u = E u$$

$$V(r) = -\frac{K e^2}{r} = -\frac{\alpha \hbar c}{r}$$



Bound states $E < 0$ (discrete)

"Free" states $E > 0$ (continuous)

Spherical symmetry $\Rightarrow u(r, \theta, \phi) = R_{El}(r) Y_{lm}(\theta, \phi)$

$$\frac{d^2}{dr^2}(r R_{El}) - \frac{l(l+1)}{r^2}(r R_{El}) = -\frac{2m}{\hbar^2} \left(E + \frac{\alpha \hbar c}{r} \right) (r R_{El})$$

Define $w(r) = r R_{El}(r)$

$$\frac{d^2 w}{dr^2} - \frac{l(l+1)}{r^2} w = \underbrace{\left(-\frac{2mE}{\hbar^2} \right)}_{\text{positive quantity (for bound states)}} w - \left(\frac{2m\alpha c}{\hbar} \right) \frac{w}{r}$$

positive quantity (for bound states)
w/units of $(\text{length})^{-2}$

Consider bound states: $E < 0$

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Multiply by $\frac{\hbar^2}{-2mE} > 0$ which has units of $(\text{length})^2$

$$\underbrace{\frac{\hbar^2}{-2mE} \frac{d^2}{dr^2} W}_{\downarrow \frac{d^2}{dp^2}} - \underbrace{l(l+1) \left(\frac{\hbar^2}{-2mEr^2} \right) W}_{\substack{\text{positive + dimensionless} \\ \rightarrow \text{call it } \frac{1}{p^2}}} = W - 2 \underbrace{\frac{m\alpha c}{\hbar} \sqrt{\frac{\hbar^2}{-2mE}}}_{\downarrow \sqrt{\frac{m\alpha^2 c^2}{-2E}}} \underbrace{\sqrt{\frac{\hbar^2}{-2mE}} \frac{1}{r}}_{\downarrow \frac{1}{p}} W$$

$$\underbrace{\sqrt{\frac{m\alpha^2 c^2}{-2E}}}_{\substack{\text{dimensionless} \\ \rightarrow \text{call it } \lambda}} \Rightarrow \boxed{E = -\frac{m\alpha^2 c^2}{2\lambda^2}}$$

$$\frac{d^2 W}{dp^2} - \frac{l(l+1)}{p^2} W = W - \frac{2\lambda}{p} W$$

$$E = -\left(\frac{1}{2}mc^2\alpha^2\right) \frac{1}{\lambda^2} = -\frac{(Ryd)}{\lambda^2} \quad (Ryd = 13.6 \text{ eV})$$

$$p = \sqrt{-\frac{2mE}{\hbar^2}} r = \sqrt{-\frac{2m}{\hbar^2} \left(-\frac{m\alpha^2 c^2}{2\lambda^2}\right)} r = \frac{m\alpha c}{\hbar \lambda} r = \frac{r}{\lambda a_0}$$

$$\text{where } a_0 = \frac{\hbar}{m\alpha c} = \text{Bohr} = 0.529 \text{ \AA}$$

$$\Rightarrow \boxed{p = \frac{r}{\lambda a_0}}$$

$$\frac{d^2 w}{dp^2} + \left[-\frac{l(l+1)}{p^2} + \frac{2\lambda}{p} - 1 \right] w = 0$$

• Solve this eqn by looking at $p \rightarrow 0$ and $p \rightarrow \infty$ limits

• Asymptotic behavior as $p \rightarrow \infty$

$$\frac{d^2 w}{dp^2} - w = 0 \Rightarrow w(p) \approx e^p, e^{-p}$$

we will solve to eqn
+ will find that its
solutions are
"well behaved"
(i.e. normalizable)
if λ is an
integer $\geq l$.

~~more generally, let $w(p) = y(p) e^{-p}$~~

• let $w(p) = y(p) e^{-p}$ for $y(p)$ some polynomial

$$w' = y' e^{-p} - y e^{-p}$$

$$w'' = y'' e^{-p} - 2y' e^{-p} + y e^{-p}$$

$$[y'' - 2y' + y] + \left[-\frac{l(l+1)}{p^2} + \frac{2\lambda}{p} - 1 \right] y = 0$$

$$y'' - 2y' + \left(\frac{2\lambda}{p} - \frac{l(l+1)}{p^2} \right) y = 0$$

$$y'' - 2y' + \frac{2\lambda}{r}y - \frac{l(l+1)}{r^2}y = 0$$

58-4

Try power series ansatz: $y = a_k r^k + a_{k+1} r^{k+1} + a_{k+2} r^{k+2} + \dots$

where a_k is the first nonvanishing coefficient ($a_0 = a_1 = \dots = a_{k-1} = 0$)
(k to be determined later)

$$y = \sum_{i=k}^{\infty} a_i r^i$$

$$y' = \sum i a_i r^{i-1}$$

$$y'' = \sum i(i-1) a_i r^{i-2}$$

$$\underbrace{\sum_{i=k} i(i-1) a_i r^{i-2}}_{\text{let } i=i'+1} - \sum_{i=k} 2i a_i r^{i-1} + \sum_{i=k} 2\lambda a_i r^{i-1} - \underbrace{\sum_{i=k} l(l+1) a_i r^{i-2}}_{i=i'+1} = 0$$

$$\sum_{i'=k-1} (i'+1) i' a_{i'+1} r^{i'-1}$$

$$\sum_{i'=k-1} l(l+1) a_{i'+1} r^{i'-1}$$

Relabel $i' \rightarrow i$ and combine the sums

$$\sum_{i=k} [(i+1) i a_{i+1} - 2i a_i + 2\lambda a_i - l(l+1) a_{i+1}] r^{i-1}$$

$$+ [k(k-1) a_k - l(l+1) a_k] r^{k-2} = 0$$

If $b(p) = \sum b_i p^i = 0$ (for all p), then $b_i = 0$ for all i

[argument by taking derivative + setting to zero]

$$[k(k-1) - l(l+1)] a_k = 0$$

If $k(k-1) \neq l(l+1)$ then $a_k = 0$

but a_k is the first nonvanishing coefficient

$$\text{so } k^2 - k - l(l+1) = 0 \Rightarrow k = l+1, -l$$

ie a_{l+1} is the first nonvanishing coefficient.

$$\left[k = -l \Rightarrow y \sim \frac{1}{p^l} \Rightarrow R \sim \frac{1}{p^{l+1}} \Rightarrow \int p^2 dp |R|^2 \sim \int \frac{dp}{p^{2l}} = \infty \text{ if } l \geq 1 \right] \begin{array}{l} \text{leads to nonnormalizable} \\ \text{wavefun} \\ \text{for } l \geq 1 \end{array}$$

For $l=0$ need to look at recursion rule

$$y(p) = a_{l+1} p^{l+1} + a_{l+2} p^{l+2} + a_{l+3} p^{l+3} + \dots$$

Also

$$[i(i+1) - l(l+1)] a_{i+1} + 2[\lambda - i] a_i = 0 \text{ for } i \geq k$$

For $l=0$,
 $k=0$
 $\Rightarrow a_0 = 0$
~~for $l=0$~~

from

For $i \geq k$,
$$a_{i+1} = \frac{-2(\lambda - i)}{[i(i+1) - l(l+1)]} a_i \quad (\text{recursion relation})$$

eg.
$$\left[\begin{aligned} a_{l+2} &= \frac{-2(\lambda - l - 1)}{2(l+1)} a_{l+1} \\ a_{l+3} &= \frac{-2(\lambda - l - 2)}{2(2l+3)} a_{l+2} \end{aligned} \right]$$
 omit $\left\{ \begin{array}{l} \text{omit } i \\ \text{omit } i \end{array} \right\}$ These are given later

etc.

So recursion relation determines all the coefficients in terms of a_{l+1} , which is determined by normalization condition

Backlog

$l=0$ is a special case

$k=0$ is a soln of $[k(k-1) - l(l+1)] a_k = 0$ for $l=0$

But then the $i=k$ eqn gives: $2\lambda a_0 = 0$

Let's go back to (setting $l=0$)

$$\sum_k i(i-1) a_i \rho^{i-2} - \sum_k 2i a_i \rho^{i-1} + \sum 2\lambda a_i \rho^{i-1} = 0$$

$\underbrace{\hspace{10em}}_{\text{vanishes for } i=0,1}$
 $\underbrace{\hspace{10em}}_{\text{vanishes for } i=0}$

so the ρ^{-1} term is just $2\lambda a_0 = 0$ ✓

go back to $y'' - 2y' + \frac{2\lambda}{\rho} y = 0$

Can see that $y \sim \cos t + a\rho + \dots$
 can't solve this unless $\lambda = 0$

so we need to start w/ $k \neq 0 \dots$

go back even further to $\nabla^2 u = -\frac{2m}{\hbar^2} (E - V(r)) u$

$l=0 \Rightarrow \frac{\partial^2}{\partial r^2} (ru) = -\frac{2m}{\hbar^2} (E - \frac{\hbar^2 c}{r}) (ru)$

Now as $r \rightarrow 0$: $ru = C + Dr \Rightarrow u = \frac{C}{r} + D$

$u \sim \frac{1}{r} \Rightarrow \nabla^2 u = \delta^{(3)}(\mathbf{r})$
 not $(\frac{1}{r^2})$

$\frac{\partial^2}{\partial r^2} (C) = -\frac{2m}{\hbar^2} (E - \frac{\hbar^2 c}{r}) C$ ← can't satisfy

the would be
 normal the
 $\sim \cos t$
 $\sim \cos t$

back up

$$0 = [k(k-1) - l(l+1)] a_k \rho^{k-2}$$

$$+ \sum_{i=k} \left([i(i+1) - l(l+1)] a_{i+1} + 2(\lambda - i) a_i \right) \rho^{i-1}$$

look at $i=k$ term

$$([k(k+1) - l(l+1)] a_{k+1} + 2[\lambda - k] a_k) \rho^{k-1}$$

$k = l+1, -l$ solve first eqn

plug $k = -l$ into 2nd

$$[(-l)(-l+1) - l(l+1)] a_{-l+1} + 2(\lambda + l) a_{-l}$$

$-2l$

$$\text{if } l=0 \Rightarrow \boxed{\lambda a_0 = 0}$$

$$\rightarrow \lambda = 0 \text{ and } l=0$$

then

$$\frac{d^2 u}{dy^2} - u = 0$$

$$\boxed{e^{-y}}$$

$$\textcircled{l=0}$$

$$y'' - 2y' + \frac{2\lambda}{\rho} y = 0$$

Consider recursion relation for large i

$$a_{i+1} \approx \frac{2i}{i(i+1)} a_i = \frac{2}{i+1} a_i$$

If this were valid for all i , then we could write

$$a_i = \frac{2^i}{i!} a_0 \Rightarrow a_{i+1} = \frac{2^{i+1}}{(i+1)!} a_0 = \frac{2}{i+1} a_i \quad \checkmark$$

Large i behavior ^(not Bohr!) determines large p behavior

$$Y(p) \xrightarrow{\text{large } p} \sum_{i=0}^{\infty} \frac{2^i}{i!} p^i a_0 = a_0 \sum_{i=0}^{\infty} \frac{(2p)^i}{i!} = a_0 e^{2p}$$

$$\text{Then } w(p) = Y(p) e^{-p} \approx e^p \quad ! \text{ nonnormalizable}$$

Loophole: this behavior can be avoided only if the series terminates at finite i

Series will terminate if λ is some integer $\geq l+1$.

Call this integer n = principal quantum number

$$\Rightarrow E_n = -\frac{(Ryd)}{n^2}, \quad n \geq l+1$$

(Bohr model prediction!)

Recursion relation:
$$a_{i+1} = \frac{-2(n-i)}{i(i+1)-l(l+1)} a_i$$

$$\Rightarrow a_{n+1} = 0$$

The only nonvanishing coeffs are $\{a_{l+1}, \dots, a_n\}$

$$y(p) = p^{l+1} \left[a_{l+1} + a_{l+2}p + \dots + a_n p^{n-l-1} \right]$$

called associated Laguerre polynomial $L_{n-l-1}^{2l+1}(2p)$

$$a_{l+2} = -\frac{(n-l-1)}{(l+1)} a_{l+1}$$

see
before

$$\left[a_{l+3} = -\frac{(n-l-2)}{(2l+3)} a_{l+2} \right] \text{ omit}$$

For example

$$n=l+1: \left. \begin{aligned} L_0^{2l+1} &= a_{l+1} \end{aligned} \right\}$$

$$n=l+2: L_1^{2l+1} = a_{l+1} \left[1 - \frac{p}{l+1} \right]$$

$$n=l+3: \left[L_2^{2l+1} = a_{l+1} \left[1 - \frac{2p}{l+1} + \frac{2p^2}{(2l+3)(l+1)} \right] \right] \text{ omit}$$

Griffiths

$$L_{n-l-1}^{2l+1}(x) \equiv -\left(\frac{d}{dx}\right)^{2l+1} \left[e^x \left(\frac{d}{dx}\right)^{n+l} [e^{-x} x^{n+l}] \right], \quad x=2p$$

Background

$$L_{n-l-1}^{2l+1}(x) = - \left(\frac{d}{dx} \right)^{2l+1} \left[e^x \left(\frac{d}{dx} \right)^{n+l} (e^{-x} x^{n+l}) \right]$$

$$L_0^{2l+1}(x) = - \left(\frac{d}{dx} \right)^{2l+1} \left[e^x \left(\frac{d}{dx} \right)^{2l+1} (e^{-x} x^{2l+1}) \right]$$

$$(-1)^{2l+1} e^{-x} (x^{2l+1} + \text{lower powers})$$

$$= \left(\frac{d}{dx} \right)^{2l+1} [x^{2l+1} + \text{lower powers}]$$

$$= (2l+1)!$$

	$l=0$	$l=1$	$l=2$	$l=3$
$n=1$	$L_0^1 = 1$			
$n=2$	$L_1^1 = -2(x-2)$	$L_0^3 = 6$		
$n=3$	$L_2^1 = 3(x^2 - 6x + 6)$	$L_1^3 = -24(x-4)$	$L_0^5 = 120$	
$n=4$	$L_3^1 = -4(x^3 - 12x^2 + 36x - 24)$	$L_2^3 = 60(x^2 - 10x + 20)$	$L_1^5 = -720(x-6)$	$L_0^7 = 5040$

$$Y(p) = p^{l+1} L_{n-l-1}^{2l+1}(2p)$$

$$W(p) = Y(p) e^{-p}$$

$$\text{But } W = r R_{El}(r) \propto \rho R_{El} \xrightarrow{n}$$

$$\begin{cases} R_{nl}(r) \sim \rho^l L_{n-l-1}^{2l+1}(2\rho) e^{-\rho} & \text{where } \rho = \frac{r}{na_0} \\ U_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{lm}(\theta, \phi) \\ E_n = -\frac{(\frac{1}{2}mc^2\alpha^2)}{n^2} \end{cases}$$

$$a_0 = \frac{\hbar}{m c \alpha} = \text{Bohr radius}$$

$$\frac{1}{2}mc^2\alpha^2 = Ryd = 13.6 \text{ eV}$$

$$\text{Since } n \geq l+1 \Rightarrow \begin{cases} n = 1, 2, 3, \dots \\ l = 0, \dots, n-1 \\ m = l, \dots, -l \end{cases}$$

$$\text{Normalization} \Rightarrow \int |U_{nlm}|^2 r^2 dr d\Omega = \int |R_{nl}|^2 r^2 dr \underbrace{\int |Y_{lm}|^2 d\Omega}_1$$

As we require

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

$$\text{units} \Rightarrow R_{nl} \sim \frac{1}{a_0^{3/2}}$$

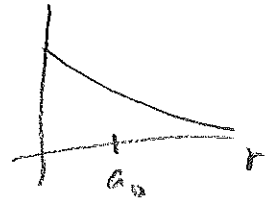
Useful $\int_0^\infty x^n e^{-x} dx = n!$

Hydrogen atom energy eigenfunctions

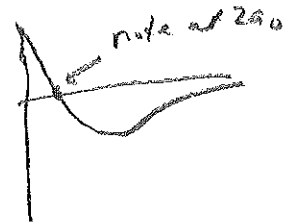
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$$\begin{matrix} \underline{m} & \underline{l} & \underline{m} & \underline{u_{nlm}(r, \theta, \phi)} \end{matrix}$$

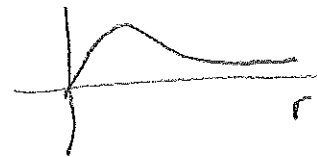
$$1s \quad 1 \quad 0 \quad 0 \quad \left(\frac{2}{a_0^3}\right) \frac{1}{\sqrt{4\pi}} e^{-\frac{r}{a_0}}$$



$$2s \quad 2 \quad 0 \quad 0 \quad \frac{1}{\sqrt{2} a_0^{3/2}} \frac{1}{\sqrt{4\pi}} \left(1 - \frac{r}{2a_0}\right) e^{-\frac{r}{2a_0}}$$



$$2p \quad 2 \quad 1 \quad m \quad \frac{1}{\sqrt{24} a_0^{3/2}} \left(\frac{r}{a_0}\right) e^{-\frac{r}{2a_0}} \begin{cases} -\sqrt{\frac{3}{8\pi}} \sin\theta e^{-1/\rho} \\ \sqrt{\frac{3}{4\pi}} \cos\theta \\ +\sqrt{\frac{3}{8\pi}} \sin\theta e^{-1/\rho} \end{cases}$$



end of course
2017, 18, 19