

Tues 15 May 07

Q11 Ch 13: Hydrogen #2

p. 363 (1)

So far we have, for  $V(r)$ ,  $\Psi = R_{\ell\ell}(r) Y_{\ell}^m(\theta, \phi)$

where  $R_{\ell\ell}(r) = \frac{U_{\ell\ell}(r)}{r}$  and  $U_{\ell\ell} \xrightarrow{r \rightarrow 0} r^{l+1}$ ,  $U_{\ell\ell} \xrightarrow{r \rightarrow \infty} e^{-\rho}$ ,  $\rho = \sqrt{2mW} \frac{r}{\hbar}$

$$(1) \left\{ \frac{d^2}{dr^2} + \frac{2m}{\hbar^2} \left[ E + \frac{e^2}{r} - \frac{\ell(\ell+1)\hbar^2}{2mr^2} \right] \right\} U_{\ell\ell} = 0 \quad (13.1.2)$$

↑  
Coulomb  $V(r)$

(13.1.7)

Now let  $rR_{\ell\ell}(r) = U_{\ell\ell}(r) = e^{-\rho(r)} V_{\ell\ell}(r)$  and try to find  $V$ .  
(2)

Sub (2) into (1) and get (13.1.8)  $\frac{d\rho}{dr} =$

$$(a) \frac{dU}{dr} = \frac{dU}{d\rho} \frac{d\rho}{dr} =$$

$$\frac{d^2U}{dr^2} = \frac{d}{dr} \left( \frac{dU}{d\rho} \right) = \frac{d\rho}{dr} \frac{d}{d\rho} \left( \frac{dU}{d\rho} \right)$$

$$(13.1.8) \quad \frac{d^2V}{d\rho^2} - 2 \frac{dV}{d\rho} + \left[ \frac{e^2 \lambda}{\rho} - \frac{\ell(\ell+1)}{\rho^2} \right] = 0 \quad \text{where } \lambda = \sqrt{\frac{2mW}{\hbar^2}}$$

Try a series solution for  $V = \rho^{l+1} \sum_{k=0}^{\infty} C_k \rho^k$   
and get recursion relations  $\frac{C_{k+1}}{C_k}$  (13.1.11)

#13.1.1 Derive 13.1.11 from 13.1.8, and 13.1.14 from

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$$\frac{C_{k+1}}{C_k}$$

$$\frac{d^2v}{dp^2} \dots$$

13.1.10

Plug  $v = \sum_{k=0}^{\infty} C_k p^{l+1+k}$  into  $\frac{d^2v}{dp^2} - 2\frac{dv}{dp} + \left[ \frac{e^{2\lambda}}{p} - \frac{l(l+1)}{p^2} \right] v = 0$

$$\frac{dv}{dp} =$$

$$\frac{d^2v}{dp^2} =$$

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

(13.1.8) becomes:

(3)

Now define  $m = k-1$ ,  $m+1 = k$ , rewrite (3):

$$0 = \sum_{\substack{k=0 \\ (k=0)}}^{\infty} C_{m+1} \{ (l+m+2)(l+m+1) - l(l+1) \} p^{l+m} + \sum_{k=0}^{\infty} C_k \{ e^{2\lambda} - 2(l+k+1) \} p^{l+k}$$

We can rename  $m$  to  $k$  and gather terms of  $p^{l+k}$  together:

$$0 = C_0 \{ (l+1)l - l(l+1) \} p^{l-1} + \sum_{k=0}^{\infty} p^{l+k} \left[ C_{k+1} \{ (l+k+2)(l+k+1) - l(l+1) \} + C_k \{ e^{2\lambda} - 2(l+k+1) \} \right]$$

$$\frac{C_{k+1}}{C_k} =$$

## Energy Levels of H-atom:

We found that  $\frac{C_{k+1}}{C_k} = \frac{-e^2 \lambda + 2l(k+l+1)}{(k+l+2)(k+l+1) - l(l+1)} \xrightarrow{k \rightarrow \infty} \frac{2}{k}$

describes  $V_{El} = \rho^{l+1} \sum_{k=0}^{\infty} C_k \rho^k \rightarrow \rho^m e^{2\rho}$

$U \sim V e^{-\rho} \sim \rho^m e^{-\rho} e^{2\rho} \sim \rho^m e^{\rho}$  must terminate at some  $k$ .

Need  $-e^2 \lambda + 2(k+l+1) = 0$  at some  $k$

(13.1.9)  $\lambda^2 = \frac{2m}{\hbar^2 W}$  : SOLVE for  $W = E(n, l, k, \rho)$

(13.1.14)  $W =$

Write this in terms of the principal quantum number  
 $n = k + l + 1$

$E_n =$

At each  $n$ , the allowed values of  $l$  are (13.1.7):

\* 13.1.3. Starting from the recursion relation, find  $\Psi_{210}$ .

$$\Psi_{\text{ellm}}(\vec{r}) = R_{\text{ell}}(r) Y_l^m(\theta, \phi) = \frac{U_{\text{ell}}(r)}{r} Y_l^m(\theta, \phi)$$

$$U_{\text{ell}}(\rho) = V_{\text{nl}}(\rho) e^{-\rho} \quad \text{where } \rho = \frac{r}{na_0} \text{ from (13.1.23) + (13.1.24)}$$

$$V_{\text{nl}}(\rho) = \sum_{k=0}^{\infty} C_k \rho^{l+k+1}$$

$$\frac{C_{k+1}}{C_k} = \frac{[-2n] + 2(k+l+1)}{(k+l+2)(k+l+1) - l(l+1)}$$

$$\left[ \text{From (13.1.11) with } \lambda = \sqrt{\frac{2m}{\hbar^2 W}} = \right.$$

(13.1.9)                      (13.1.16)

$$\text{So } e^{-\lambda r} =$$

$$= 2n \quad ]$$

$$\Psi_{210} : l = \underline{\quad} \quad m = \underline{\quad}$$

$$\frac{C_1}{C_0} =$$

Therefore all  $C_k = 0$  except  $C_0$ . Just leave  $C_0$  as an unknown constant for now.

$$V_{21}(\rho) =$$

$$U_{21}(r) =$$

Normalizing  $\Psi_{210}$ : The normalization condition on  $U_2(r)$

is

$$1 = \int_0^{\infty} (U_2(r))^2 dr =$$

Special integral:  $\int_0^{\infty} r^4 e^{-r/a_0} dr = (4!) a_0^5$  ( Dwight 860.07)

Find  $C_0 =$

$$= \sqrt{\frac{2}{3a_0}}$$

Finally  $\Psi_{210}(r, \theta, \phi) =$

$$\Psi_{210}(r, \theta, \phi) = \sqrt{\frac{1}{32\pi a_0^2}} \left(\frac{r}{a_0}\right) e^{-r/2a_0} \cos\theta$$

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QM QUESTION - Why construct  $L_{\pm} = L_x \pm iL_y$ ?

Recall that for QHO we constructed  $a_{\pm} = A(\mp ip + m\omega x)$  because we sought eigenstates & eigenvalues for

$$H\psi = \left( \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} \right) \psi \quad \text{Griffiths QM p. 42}$$

$$E\psi = \frac{1}{2m} (p^2 + (m\omega x)^2) \psi$$

We'd like to be able to factor  $H = \frac{1}{2m} (p^2 + (m\omega x)^2)$   
 $u^2 + v^2$

If  $p$  &  $x$  weren't operators, we could just use  $u^2 + v^2 = (iu+v)(-iu+v)$

This motivates us to construct  $a_{\pm} = A(\mp ip + m\omega x) \dots$   
 $[x, p] = i\hbar$

Similarly, when seeking simultaneous eigenstates of the angular momentum operators  $L^2$  and  $L_z$

Shankar p. 330 (1)

$$L^2 |\alpha\beta\rangle = \alpha |\alpha\beta\rangle \quad \text{and} \quad L_z |\alpha\beta\rangle = \beta |\alpha\beta\rangle$$

$\uparrow$  value state                       $\uparrow$  value state

Use  $L^2 = L_z^2 + L_x^2 + L_y^2$  to write

$$(L^2 - L_z^2) |\alpha\beta\rangle = (\alpha - \beta) |\alpha\beta\rangle = (L_x^2 + L_y^2) |\alpha\beta\rangle = u^2 + v^2$$

By analogy with  $a_{\pm}$ ,

(12.5.3) This motivates us to construct  $L_{\pm} = L_x \pm iL_y \dots$   
 $[L_x, L_y] = i\hbar L_z$