# 7. Hydrogen Atoms,4

# lecture 27, October 32, 2017

I crack myself up sometimes

# housekeeping

I got nothin'



# today

# Hydrogen atom, more





WHERE WE WERE ! Schrodinger equation for 3 dimensional configuration  $-\frac{\hbar^{2}}{2\mu}\left(\frac{1}{r^{2}}\frac{\partial}{\partial r}\left(r^{2}\frac{\partial}{\partial r}\right) + \frac{1}{r^{2}\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^{2}\sin^{2}\theta}\frac{\partial^{2}}{\partial\theta^{2}}\Psi(r,\theta,\phi)$ - <u>e</u> 4(r, 6, q) = E4(r, 6, q) 446.r reduced WASS  $R_{nk}(r) = -\left[\left(\frac{2}{na_{o}}\right)\frac{(n-k+1)!}{2n\left[(n+k)\right]^{3}}\right]^{\frac{1}{2}}\left(\frac{2r}{na_{o}}\right)^{\frac{1}{2}} - \frac{r'}{na_{o}}\frac{2k+1}{n+k}\left(\frac{2r}{na_{o}}\right)$  $\Upsilon_{nlm_{\ell}}(r, \theta, \phi) = R_{nl}(r) \Upsilon_{l}^{m_{\ell}}(\theta, \phi)$  $E_n = \underbrace{e^4}_{(4\pi6)} \underbrace{\mu}_{522n^2}$ "eigenvalves" "eigenfunctions"

GUANTUM NUMBERS of the QUANTUM CENTRAL FORCE SOLUTION

Principle Quantum Number N:

n=1,2,3.....

Orbital Angular Momentum Quantum Number



Maquetic Quantum Number

$$-2 \leq m_{L} < 2$$



a fern: 12m

$$Y_0^0( heta,arphi)=rac{1}{2}\sqrt{rac{1}{2}}$$

I = 1<sup>[1]</sup> [edit]

I = 2<sup>[1]</sup> [edit]

$$\begin{split} &|=\mathbf{3}^{[1]} \quad [\operatorname{edit}] \\ &Y_{3}^{-3}(\theta,\varphi) = \frac{1}{8}\sqrt{\frac{35}{\pi}} \cdot e^{-3i\varphi} \cdot \sin^{3}\theta \quad = \frac{1}{8}\sqrt{\frac{35}{\pi}} \cdot \frac{(x-iy)^{3}}{r^{3}} \\ &Y_{3}^{-2}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{105}{2\pi}} \cdot e^{-2i\varphi} \cdot \sin^{2}\theta \cdot \cos\theta \quad = \frac{1}{4}\sqrt{\frac{105}{2\pi}} \cdot \frac{(x-iy)^{2}z}{r^{3}} \\ &Y_{3}^{-1}(\theta,\varphi) = \frac{1}{8}\sqrt{\frac{21}{\pi}} \cdot e^{-i\varphi} \cdot \sin\theta \cdot (5\cos^{2}\theta - 1) \quad = \frac{1}{8}\sqrt{\frac{21}{\pi}} \cdot \frac{(x-iy)(4z^{2} - x^{2} - y^{2})}{r^{3}} \\ &Y_{3}^{-1}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{7}{\pi}} \cdot (5\cos^{3}\theta - 3\cos\theta) \quad = \frac{1}{4}\sqrt{\frac{7}{\pi}} \cdot \frac{z(2z^{2} - 3x^{2} - 3y^{2})}{r^{3}} \\ &Y_{3}^{-1}(\theta,\varphi) = -\frac{1}{8}\sqrt{\frac{21}{\pi}} \cdot e^{i\varphi} \cdot \sin\theta \cdot (5\cos^{2}\theta - 1) \quad = -\frac{1}{8}\sqrt{\frac{21}{\pi}} \cdot \frac{(x+iy)(4z^{2} - x^{2} - y^{2})}{r^{3}} \\ &Y_{3}^{-1}(\theta,\varphi) = -\frac{1}{8}\sqrt{\frac{21}{\pi}} \cdot e^{i\varphi} \cdot \sin\theta \cdot (5\cos^{2}\theta - 1) \quad = -\frac{1}{8}\sqrt{\frac{21}{\pi}} \cdot \frac{(x+iy)(4z^{2} - x^{2} - y^{2})}{r^{3}} \\ &Y_{3}^{-1}(\theta,\varphi) = -\frac{1}{4}\sqrt{\frac{105}{2\pi}} \cdot e^{2i\varphi} \cdot \sin^{2}\theta \cdot \cos\theta \quad = \frac{1}{4}\sqrt{\frac{105}{2\pi}} \cdot \frac{(x+iy)^{2}z}{r^{3}} \\ &Y_{3}^{-1}(\theta,\varphi) = -\frac{1}{8}\sqrt{\frac{35}{\pi}} \cdot e^{3i\varphi} \cdot \sin^{3}\theta \quad = -\frac{1}{8}\sqrt{\frac{35}{\pi}} \cdot \frac{(x+iy)^{3}}{r^{3}} \end{split}$$

I = 4<sup>[1]</sup> [edit]

$$\begin{split} Y_4^{-4}(\theta,\varphi) &= \frac{3}{16}\sqrt{\frac{35}{2\pi}} \cdot e^{-4i\varphi} \cdot \sin^4 \theta = \frac{3}{16}\sqrt{\frac{35}{2\pi}} \cdot \frac{(x-iy)^4}{r^4} \\ Y_4^{-3}(\theta,\varphi) &= \frac{3}{8}\sqrt{\frac{35}{\pi}} \cdot e^{-3i\varphi} \cdot \sin^3 \theta \cdot \cos \theta = \frac{3}{8}\sqrt{\frac{35}{\pi}} \cdot \frac{(x-iy)^3 z}{r^4} \\ Y_4^{-2}(\theta,\varphi) &= \frac{3}{8}\sqrt{\frac{5}{2\pi}} \cdot e^{-2i\varphi} \cdot \sin^2 \theta \cdot (7\cos^2 \theta - 1) = \frac{3}{8}\sqrt{\frac{5}{2\pi}} \cdot \frac{(x-iy)^2 \cdot (7z^2 - r^2)}{r^4} \\ Y_4^{-1}(\theta,\varphi) &= \frac{3}{8}\sqrt{\frac{5}{\pi}} \cdot e^{-i\varphi} \cdot \sin \theta \cdot (7\cos^3 \theta - 3\cos \theta) = \frac{3}{8}\sqrt{\frac{5}{\pi}} \cdot \frac{(x-iy) \cdot z \cdot (7z^2 - 3r^2)}{r^4} \\ Y_4^{-1}(\theta,\varphi) &= \frac{3}{16}\sqrt{\frac{1}{\pi}} \cdot (35\cos^4 \theta - 30\cos^2 \theta + 3) = \frac{3}{16}\sqrt{\frac{1}{\pi}} \cdot \frac{(35z^4 - 30z^2r^2 + 3r^4)}{r^4} \\ Y_4^{1}(\theta,\varphi) &= \frac{-3}{8}\sqrt{\frac{5}{\pi}} \cdot e^{i\varphi} \cdot \sin \theta \cdot (7\cos^3 \theta - 3\cos \theta) = \frac{-3}{8}\sqrt{\frac{5}{\pi}} \cdot \frac{(x+iy) \cdot z \cdot (7z^2 - 3r^2)}{r^4} \\ Y_4^{2}(\theta,\varphi) &= \frac{3}{8}\sqrt{\frac{5}{2\pi}} \cdot e^{2i\varphi} \cdot \sin^2 \theta \cdot (7\cos^2 \theta - 1) = \frac{3}{8}\sqrt{\frac{5}{2\pi}} \cdot \frac{(x+iy) \cdot z \cdot (7z^2 - 3r^2)}{r^4} \\ Y_4^{3}(\theta,\varphi) &= \frac{-3}{8}\sqrt{\frac{35}{2\pi}} \cdot e^{3i\varphi} \cdot \sin^3 \theta \cdot \cos \theta = \frac{-3}{8}\sqrt{\frac{3}{\pi}} \cdot \frac{(x+iy)^3 z}{r^4} \\ Y_4^{4}(\theta,\varphi) &= \frac{3}{16}\sqrt{\frac{35}{2\pi}} \cdot e^{4i\varphi} \cdot \sin^4 \theta = \frac{3}{16}\sqrt{\frac{35}{2\pi}} \cdot \frac{(x+iy)^4}{r^4} \end{split}$$



Nounclization:  $1 = \left( \left( \left( |R(r)|^2 |Y(0, 6)|^2 r^2 dr \sin \theta d\theta d\varphi \right) \right)^2 \right)^2 \left( |R(r)|^2 |Y(0, 6)|^2 r^2 dr \sin \theta d\theta d\varphi \right) \right)^2$ all space  $1 = \left( \frac{\pi}{|2(r)|^2} dr \right) \left( \frac{\pi}{|Y(\theta, \varphi)|^2} \right) \frac{\pi}{|Y(\theta, \varphi)|^2} \frac{1}{|Y(\theta, \varphi$ can sort of visualize 2 different propamility distributions:  $r^2|R(r)|^2dr$ 1Yem (Q. p) Sinddodep

Most prohable? In hydrogen, z=1  $P_{10} = 4 r^2 e$   $R_{10} = 4 r^2 e$  $\frac{dP_{10}(r)}{dr} = \frac{4}{G_0^3} \left[ 2re - r^2 \left( \frac{2r}{A_0} \right) e^{-2r/A_0} \right]$ O for extremum - $= \frac{4}{6a^3} e^{-\frac{2v}{6a}} \left[ \frac{2v}{2v} - \frac{2r^2}{6a} \right]$ " r=a. How eool is THAT? =) most probable P10 0.6 Pio Bohr seid 0.3 r/a. r/a. 10 2 10 2 4 4

Average "place" for electron ?  $\langle r \rangle = \begin{pmatrix} ob \\ r P_{10}(r) b r = 4 \\ a_{3}^{3} \end{pmatrix} \begin{pmatrix} cb \\ r^{3}e \\ dr \end{pmatrix}$ lhe  $\int z^n e^{-z} dz = h!$ Charge varichles: z = 21/au -most probable  $\langle v \rangle = \frac{a_o}{4} (3!) P_{io} \quad a_{i} = \frac{a_i}{4}$ 0.3  $\langle v \rangle = 3a_0$ r/a. 10 2 WHERE IS THE ELECTRON?

Average "place" for electron ?  $\langle r \rangle = \begin{pmatrix} ob \\ r P_{10}(r) b r = 4 \\ a_{3}^{3} \end{pmatrix} \begin{pmatrix} cb \\ r^{3}e \\ dr \end{pmatrix}$ lhe  $\int z^n e^{-z} dz = h!$ Charge variches: z = 21/au -most probable  $\langle v \rangle = \frac{a_o}{4} (3!) P_{io} a_6 - \frac{1}{4}$ 0.3  $\langle v \rangle = \frac{3}{2}a_{o}$ r/a. 10 2 WHERE IS THE ELECTRON?



Pruhahi hity of electron outside the 1st Bohr orbit? assume: 15  $P(r>a_{o}) = \int_{-\infty}^{\infty} P_{io}(r) dr$  $= \frac{4}{a_3} \int_{a_0}^{\infty} r^2 e^{-2r/a_0} dr$ another one of more integrals  $\int x^{L} e^{-x} dx = -\frac{1}{2} (x^{L} + 2x + 2) e^{-x}$ = { x²e dx X= ZV/a. P(v)a.) = 5e<sup>-2</sup>~ 0.68 => 2/3 of the time ! How chout clearly outside of its atom? >1= 100 a. P(~>10×46)= 10 7 O

How chout 2s state ... Yo -> symmetril.  $R_{20} = \frac{1}{\sqrt{(2q_0)^3}} \left( 2 - \frac{r}{q_0} \right) e$ -r/200 density peaks 0.4 1s $4\pi r^2 \cdot \psi^2$ 0.3 -2s electrons grand a significant time in 1s land 0.2 2s0.1 3*s* 500 700 900 1100 100 300 1300 1500 *r* (pm)







TRANSITIONS ... the almost real way "Oscillates" A e Br / lin an P Or / oscillating electric dipote m external. radiation or courin ous p=er YA (r, d, q) & YB (r, d, q) each wave functions for "levels" A Z B -> for a transition, they must "overlap" in the "presence" of an electric dipole operator.  $\langle p \rangle = \int \int \Psi_{A}^{*}(r, 0, \varphi) q\hat{r} \Psi_{B}(r, 0, 6) r^{2} dr sin \theta d\theta d\phi$ If integrals are zero => no transition from B + A non-zero => transitions from B + A can happen & calculation yields prob & rate (intensities)

 $(p) = \int r^2 R(r)_A^* R(r)_B dr \int \left( Y_{\ell_A}^{M_{\ell_A}}(\theta, \phi) Y_{\ell_B}^*(\theta, \phi) \sin \theta d\theta d\phi \right)$ compricated ... cound the allowed " and " for bidden" but always non-zero transitions I which becaue particular Al's always Al= ±1 so: p->s? sure S-> S, P-> D ... ? hope "selection Rules" + ut quite



Orbiting electric charges -> a magnetic moment. 4 pi current loop Classical E & M : magnetic moment |µ| = IA (R.H. rule)  $T = \frac{dQ}{dt} = \frac{Q}{T}$ If an electric charge going in a circle  $L = mvr + v = 2\pi r + A = \pi r^2$ 50  $L = m \left( \frac{2\pi r}{T} \right) r = 2m \frac{\pi r^2}{T} = 2m \frac{A}{T}$ h = IA = QA = QL N  $\vec{\mu} = Q\vec{L}$ Zm ZmThe= - e I

Strange superposition of classical & quantum mechanical votions: We found. L= trve(l+1) w/ quantized projection onto Lz axis - Lz = met a vector we have no prefared direction ... I could be anywhere something must pith a particular direction and break that symmetry & define the "axis of quantization" Magnetic fields do that.



 $\mu_{B} = e\hbar = 9.3 \times 10 J/T$ My= -e time defines Bohr Magneton atomic magnetic mounts can be Mz=-MBML  $\Rightarrow$ Throught of as multiples of MB. -> seeks to align in and 3 T = M×B Remember:  $\vec{\tau} = d\vec{L} = \vec{Q} \cdot \vec{L} \times \vec{B}$  $dt = \vec{Z} \cdot \vec{M}$ 

4 B de perpendicular to plane of BEE IdLI = Lsmtdp d6= Idll Lsint LSMO  $\frac{|dL|}{dk} = T$  $d\phi = |\tau| dt$ Lsin  $\theta$ do = Q/2m (LBsin 0) dt LSint  $d\phi = \frac{BQ}{2m}dt$ => precession@ angular frequency:  $\omega_{L} = \frac{d\phi}{dt} = \frac{QB}{ZM}$ Larmor Frequency

BUT ... M is quantized according to Lz ply = - MB Me l=1, for example :-ML O from V = - I. B V is indeed quantized The magnetic field defines a particular direction in space -> the quantization axis, along B ... 3  $V = \underbrace{e}_{2m} \overrightarrow{L} \cdot \overrightarrow{B} = e |B| L_{3}$ me ranges over - l -> + l V=MBMLB



"NORMAL ZEEMAN EFFECT 1 -> 3 splitting \_\_ "normal" because classical proture predicts Vough behavior "ANOMALOUS" ZEEMAN EFFECT 1 -> 4 ov } experimentally confusing, classically, disturbing 1-76 "Stern-Gerlach Experiment" \_> slides!

### 'Spin<u>"</u>

sometimes we use "normal language"

to refer to a physical property without a common-sense analog

and sometimes, just to be silly

#### Remember a current loop: where's the B field?



called a "magnetic dipole"

Like a bar magnet, with the north pole up...

Remember that Oersted found that a compass needle followed the B field, so this setup would also

external B field



## dipole moment

characterizes the magnetism of a current loop

#### A current loop's magnetism can be characterized



more current, higher the moment – the  $\mu$  the more torque

external B field

μ

Bohr was not the whole story

but his quantization condition was mostly correct Orbital angular momentum - the s, p, d, f, g, h, etc originates with Schroedinger's evolution of Bohr's original idea:  $L = mvr = \frac{nh}{2\pi}$ 

 $L_z = m_\ell \frac{h}{2\pi}$ 

= 0: s = 1: p = 2: d

Β, μ

In Schroedinger's model

1)

But, the electron's orbit is a little current

So, atomic orbits should twist

external B field

μ

emember spectroscopic notation

from Chemistry?

That's what Otto Stern and Walther Gerlach set about to measure in 1922...



he Bohr Model predicted a bunch of pots

since Silver is a complicated atom:

1s<sup>2</sup> 2s<sup>2</sup> 2p<sup>6</sup> 3s<sup>2</sup> 3p<sup>6</sup> 3d<sup>10</sup> 4s<sup>2</sup> 4p<sup>6</sup> 4d<sup>10</sup> 5s<sup>1</sup>



If Bohr was right

## Whattheyswyong



Separation into 2 spots evidence of "quantization" of some sort...why 2?

Separation into 2 locations, which made no sense.

Something is "quantized"

you can't always do what you're supposed to do

> young Dutch experimenters George Uhlenbeck\* and Sam Goudsmit had an idea

told by their advisor "don't publish"

they did.

\* eventually professor at UofM

The electron is *like* a spinning charge...



Like for orbital angular momentum,

$$L_z = m_\ell \frac{h}{2\pi}$$

Electrons have an **intrinsic** angular momentum

$$S_z = m_s \frac{h}{2\pi}$$

But, the "spin" can only take on two values:

$$m_s = +rac{1}{2}$$
 or  $m_s = -rac{1}{2}$ 

We say "spin, plus 1/2" or "spin up" and "spin, minus 1/2" or "spin down"

Stern & Gerlach got a hodge - podge of results Oxygen 2s22p4 5 spots Silver 2 spots --- 55 Interpreted as an augular - moventum - like selection rule of "1" = 1/2 You're not much if you're not Dutch ... Govdsmit & Uhlenbech provosed electron has an inhaest property , "spin" S= 1/2 with projections like L: 151= tr VS(S+i) Sz 1/2th 1 2 5 = 51/2.3/2 [S] = 13 h - 1/2th - $S_2 = \pm 1/2h = m_s h$ 

Spin

has features like angular nomention -- waquetic - like

NO CINCULAR CURLENTS!

NO CHARGES GOING AMOUND ANY THING !

NOT A BALL OF CHAMLE ROTATING !



#### SPIN IS INHERENT TO ELECTRONS

lousy name!

no-thing is "spinning"

DEFINE AN ELECTRON!

- · An excitation of the electron field
- · having wass = 0.51 Nev/c2
- · having electric charge = -1.6×10<sup>-19</sup>C
- · having intrinsic spin = 1/2

Magnetic Moment  $\vec{\mu}_s = -g_e \stackrel{e}{=} \vec{s}$  $\sum_{zme}$ a fudge factor .- measurable: gyromagnetic ratio (stay tuned) No reason or "implementation" of spin in Wilsontrue Mechanics Until 1928: Paul Dirac -> first relativistic quantum mechanics The Dirac Equation designed to deal with negative E · 4 wave functions resulted spin falls ( 2) with + energies -> electron 2) with - everyies -> auti-electron out from momentizs Spin is an inherently Relativistic property of electrons ...

... and neutrons, protons -> all "fermions" Also a quantum mechanics of integer-spin excitations -> all "bosons" 5=0 pions, kaons, Higgs boson .... puston, vho meson, W, Z\_\_\_ 5=1  $\Delta l = \pm 1$ that's why Angular momentum is conserved .- & radiates away and takes angular momentum of to from system So , Al is reduced.

ABOUT q.

We have 2 moments uns:

Ovinital avendar momentum:  $\vec{\mu}_{\ell} = -\frac{\mu_{\mathcal{B}}}{\hbar}\vec{L} \left( = -\frac{q_{\ell}\mu_{\mathcal{B}}\vec{L}}{\hbar} \right)$ 

 $\vec{\mu}_{S} = -2\mu_{B}\vec{S}\left(=-g_{S}\mu_{B}\vec{S}\right)$ Spin "intrincic" angular momentum:

gs is strictly a relativistic quantity.

gi=1

ge is constines included.



Contributions and up and wodity static properties of the electron  $\overline{\mu}_{s}(e) = g_{e} \stackrel{e}{=} \stackrel{\vec{s}}{\underline{s}}$ I net effect is to wording g= 2 "q-2" \_. " que minus two" \_... a vace for precision between themy (~10° individual Feynman diagrams) and experiment ( heroic Penning Trap experiments )