A bit on quantum mechanics and atomic physics

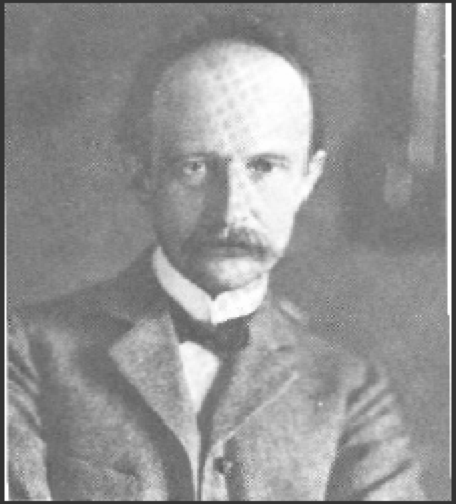
Physics 114

Spring 2006 – S. Manly

References and photo sources:

K. Krane, Modern Physics, John Wiley and Sons, 1983

Three of the players



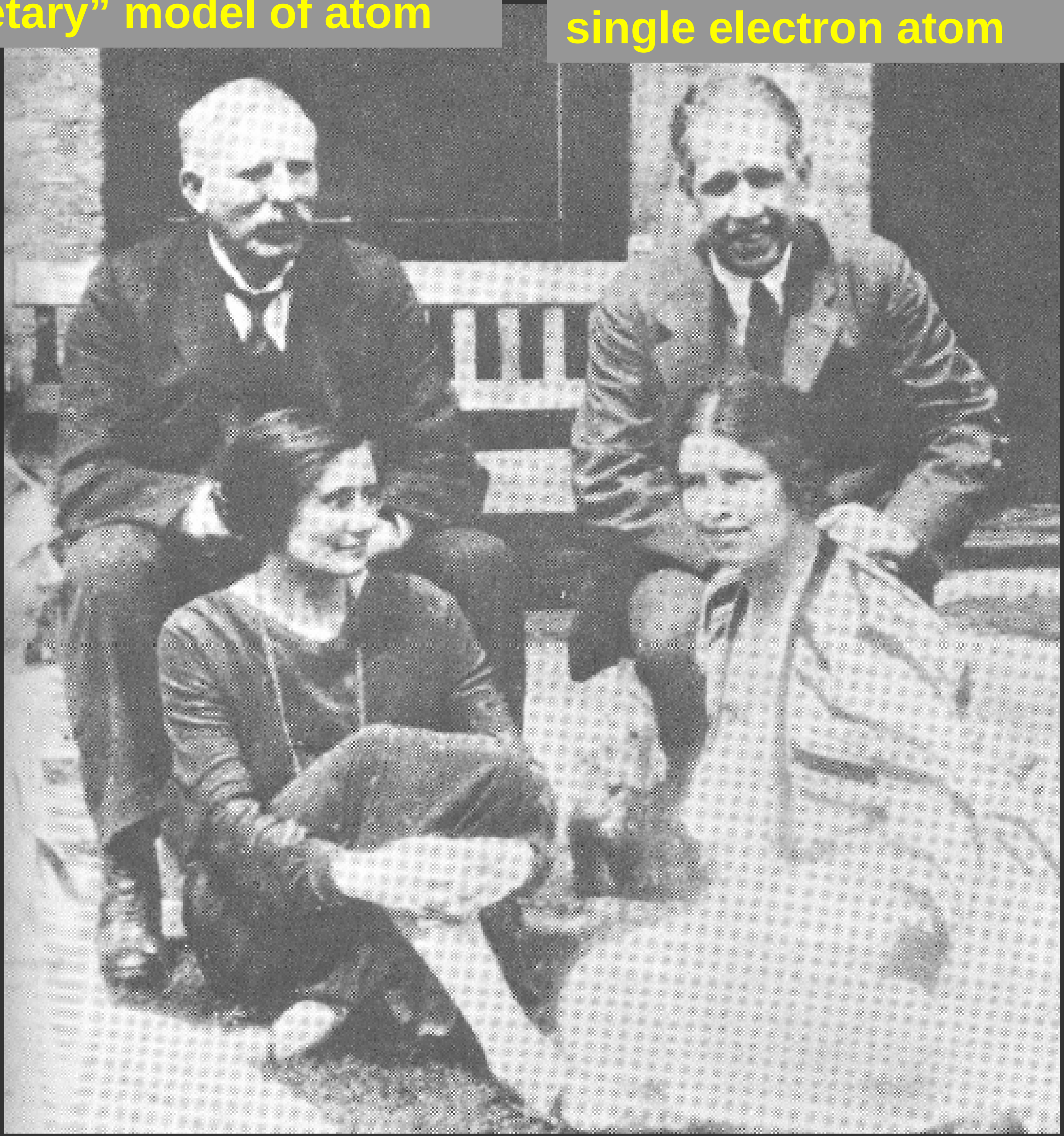
Max Planck (1858-1947) – 1918 Nobel Prize for work on spectral distribution of radiation (blackbody radiation)

Louis deBroglie (1892-1987) First suggested matter has wavelike properties

Erwin Schrodinger (1887-1961) – Developed mathematical theory of wave mechanics that permitted the calculation of physical systems

Earnest Rutherford (1871-1937)
nuclear “plantetary” model of atom

Niels Bohr (1885-1962) developed a semi-classical nuclear model of the single electron atom



Time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\,\psi(x) = E\,\psi(x)$$

$\leftarrow$ KE Term $\leftarrow$ PE Term $\leftarrow$ TOT E

$\psi(x) \equiv$ Wave function of particle

What is $\psi(x)$?

$|\psi(x)|^2 dv$ = prob. of finding particle in volume dv

$$\int_{\text{All SPACE}} |\psi(x)|^2 dv = 1$$ particle is someplace

Sub in V as appropriate + solve

for H Atom

p e^-

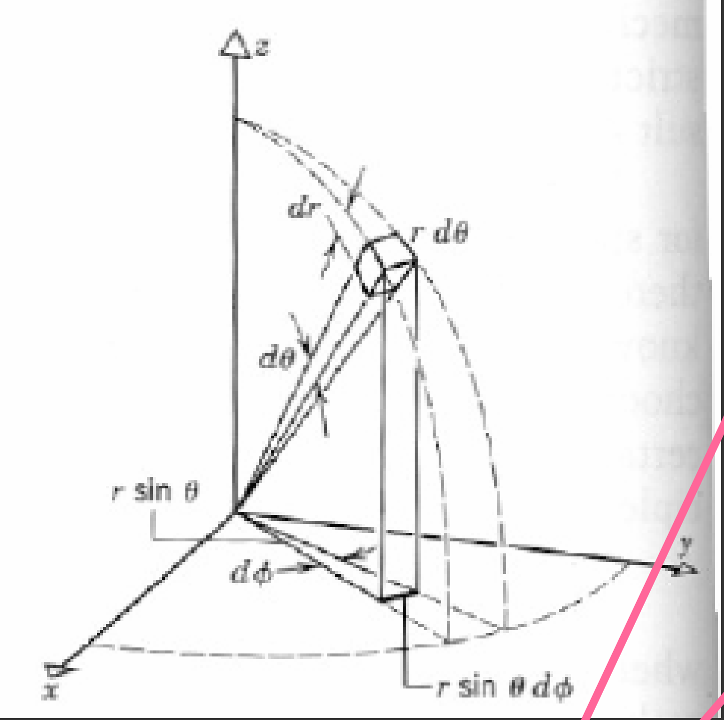
Must generalized to 3d, spherical coordinates

$$V(r) \longrightarrow \frac{1}{4\pi\epsilon_0}\frac{|q|^2}{r^2}$$ + Solve

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial \psi(r)}{\partial r} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 \psi(r)}{\partial \phi^2} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \psi(r)}{\partial \theta}\right)\right.$$

$$+ \frac{1}{4\pi\epsilon_0}\frac{|e|^2}{r^2}\psi(r) = E\,\psi(r)$$

Now solve



Separates into r, θ, Φ eqns

Energy or principal quantum number

n = 1, 2, 3 …

Orbital quantum number

l = 0, 1, … n-1

Magnetic quantum number

-l, -|l-1|, …, 0, 1, … l-1, l

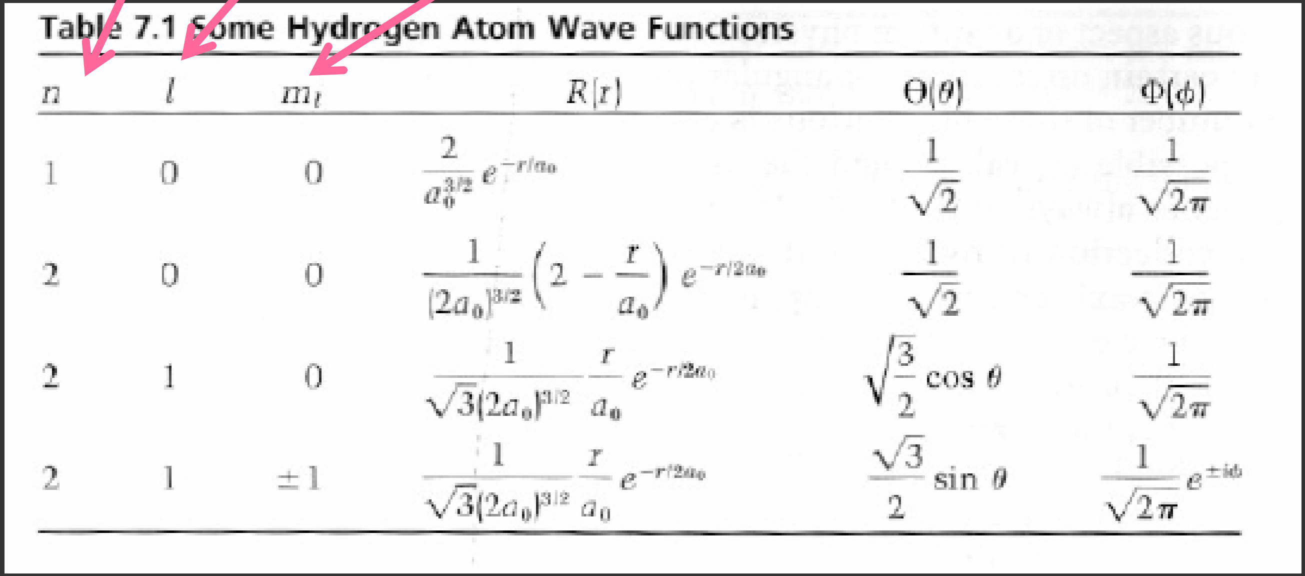
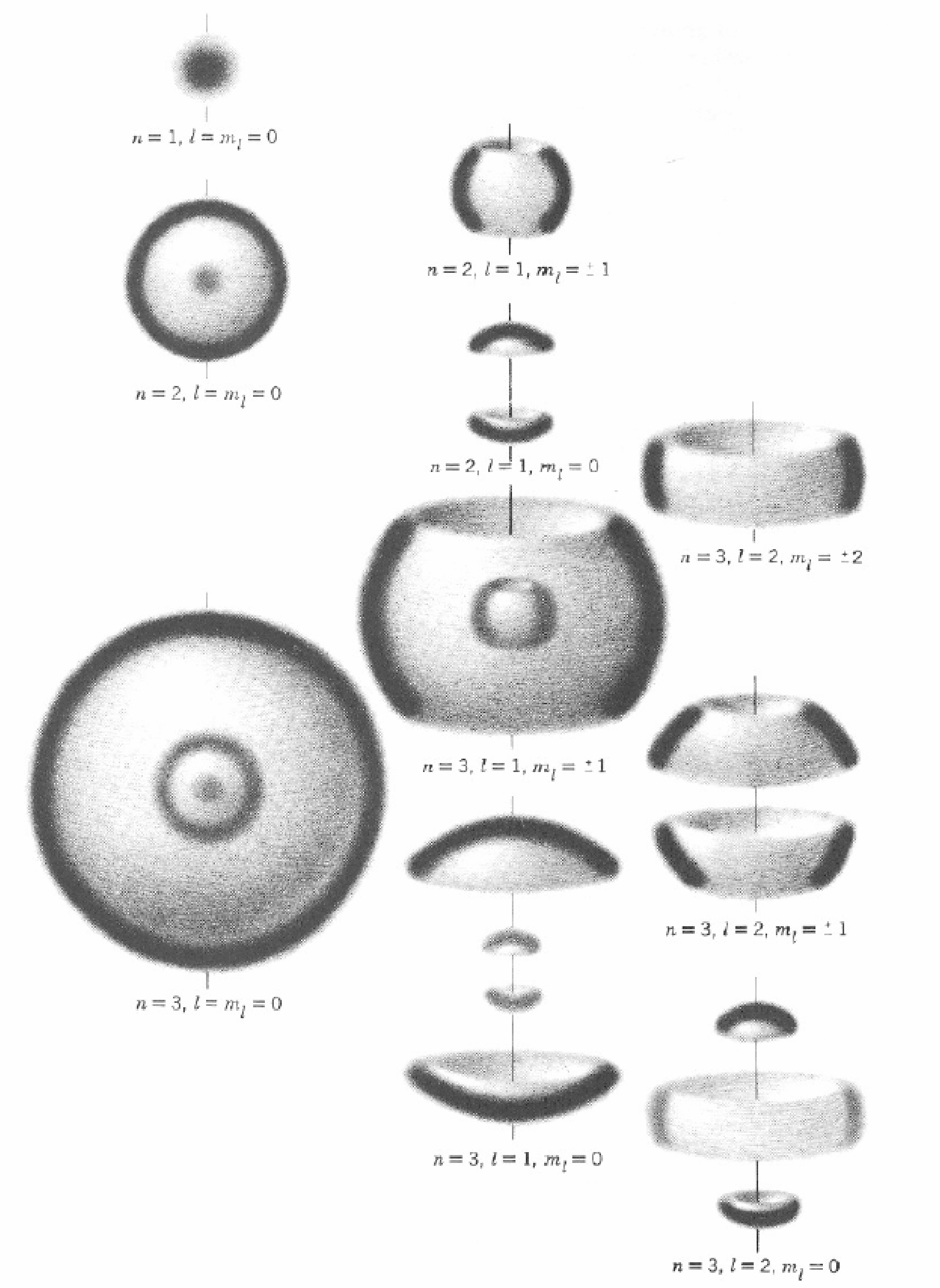


Table 7.1 Some Hydrogen Atom Wave Functions

n	l	m_l	$R(r)$	$\Theta(\theta)$	$\Phi(\phi)$
1	0	0	$\frac{2}{a_0^{3/2}} e^{-r/a_0}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2\pi}}$
2	0	0	$\frac{1}{(2a_0)^{3/2}}\left(2-\frac{r}{a_0}\right) e^{-r/2a_0}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2\pi}}$
2	1	0	$\frac{1}{\sqrt{3}(2a_0)^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$	$\sqrt{\frac{3}{2}} \cos\theta$	$\frac{1}{\sqrt{2\pi}}$
2	1	± 1	$\frac{1}{\sqrt{3}(2a_0)^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$	$\frac{\sqrt{3}}{2} \sin\theta$	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$

Probability distributions for several allowed atomic states for the 1-electron atom

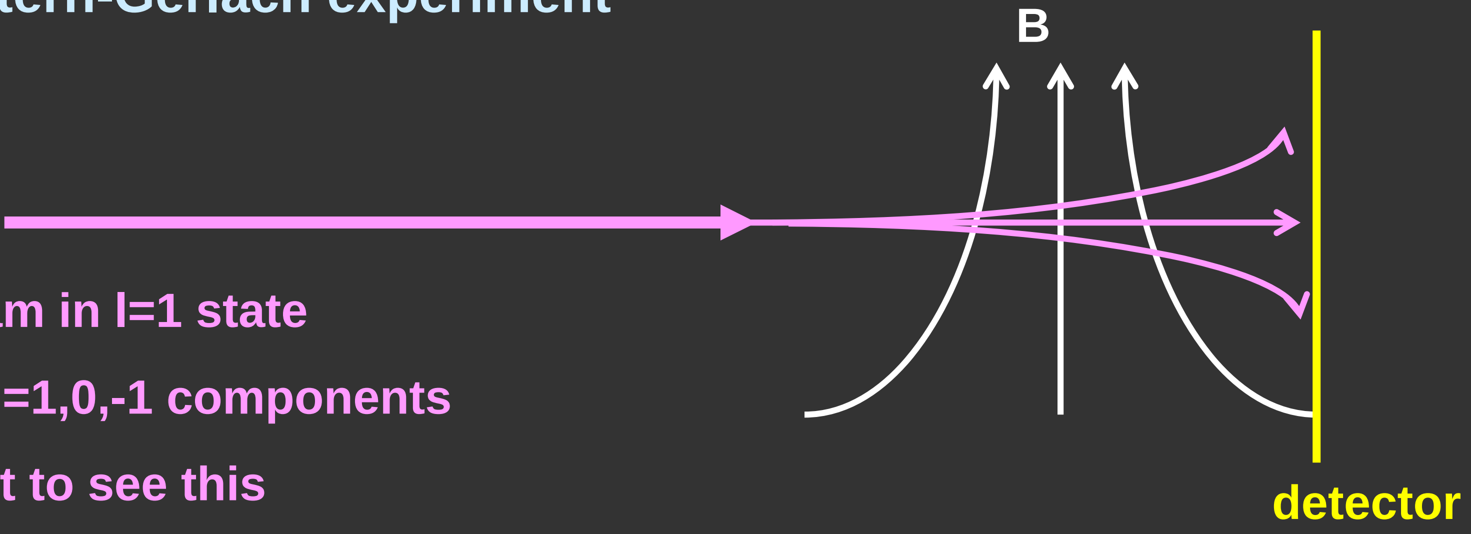
Increasing n adds new radial layers, l=0 give spherical symmetry, l not 0 brings in angular dependence



General Quant. Mech. result regarding force on magnetic dipole in a non-uniform magnetic field

$$\vec{F}_z = \frac{\partial B_z}{\partial z} |\vec{\mu}_z| = \frac{\partial B_z}{\partial z} m$$

Stern-Gerlach experiment



e- beam in l=1 state

has m=1,0,-1 components

expect to see this

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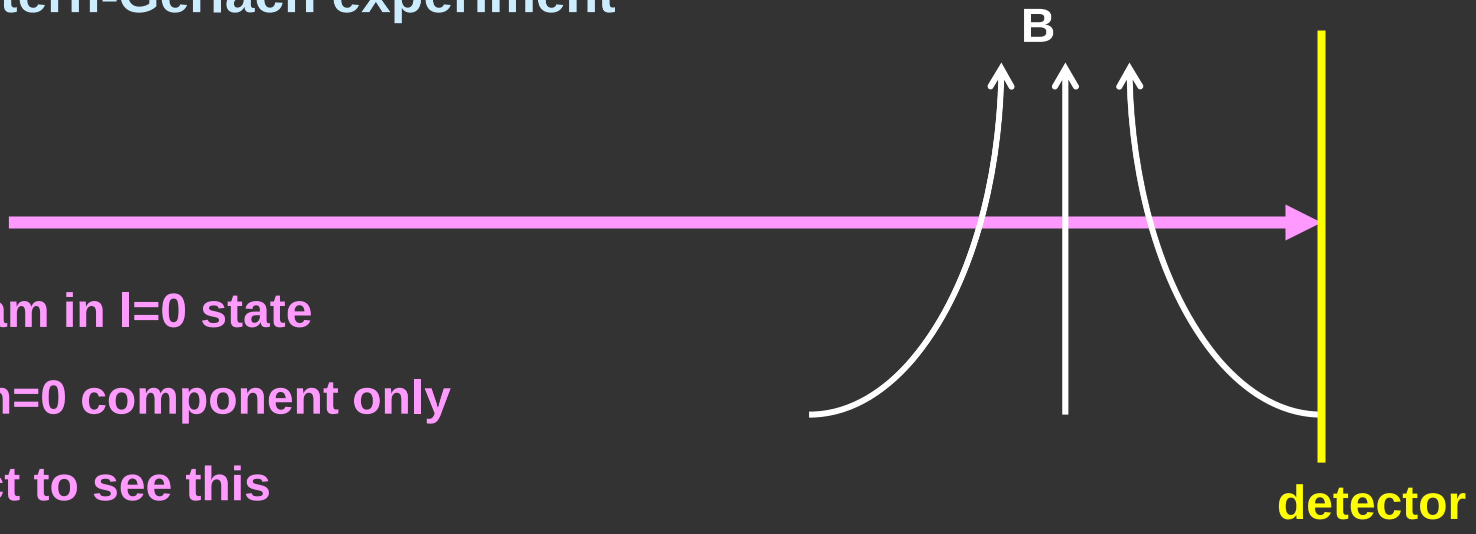


e- beam in l=0 state

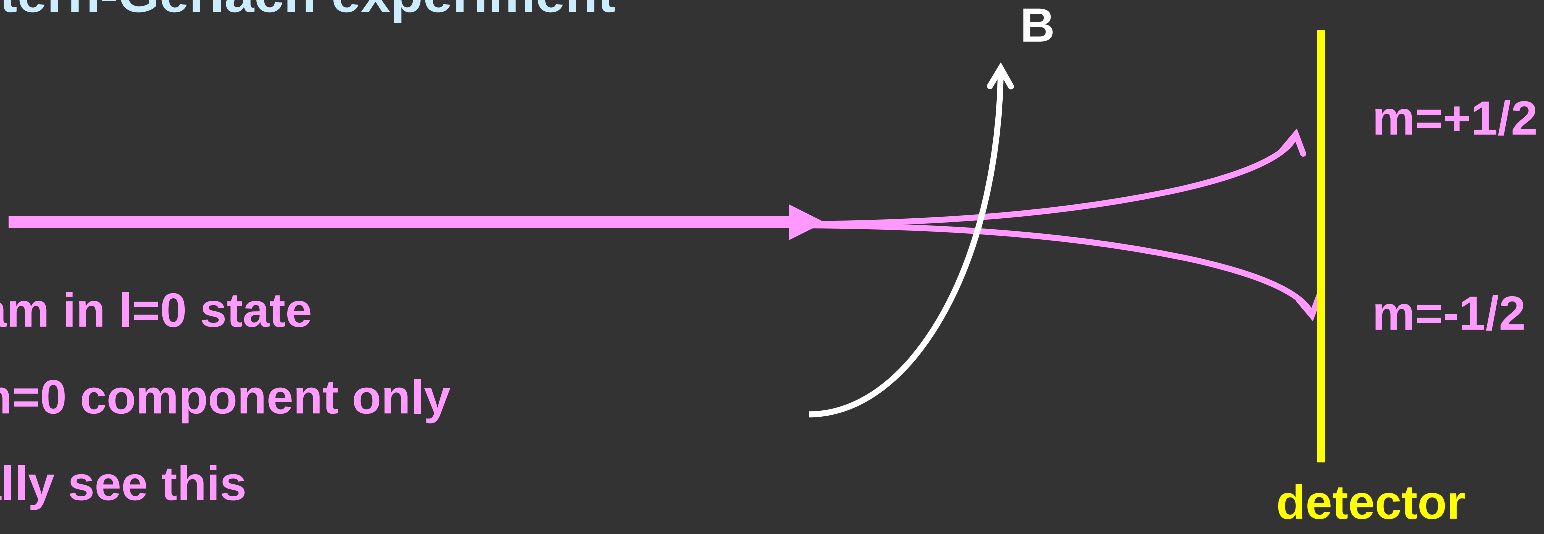
Has m=0 component only

expect to see this

SURPRISE! … fundamental particle have an intrinsic magnetic moment. Call it spin.

$$\vec{F}_z = \frac{\partial B_z}{\partial z} |\vec{\mu}_z| = \frac{\partial B_z}{\partial z} m$$

Stern-Gerlach experiment



e- beam in l=0 state

Has m=0 component only

Actually see this

Intrinsic spin - two varieties

Huge effect on
multi-electron
atoms

Fermions = half integral spin, such as 1/2, 3/2, 5/2, … , 73/2 …

protons, neutrons, electrons are all fermions (s=1/2)

no two fermions can occupy the same exact quantum state

Bosons = integral spin, such as 0, 1, 2 …

photons (s=1) and pions (s=0) are examples of bosons

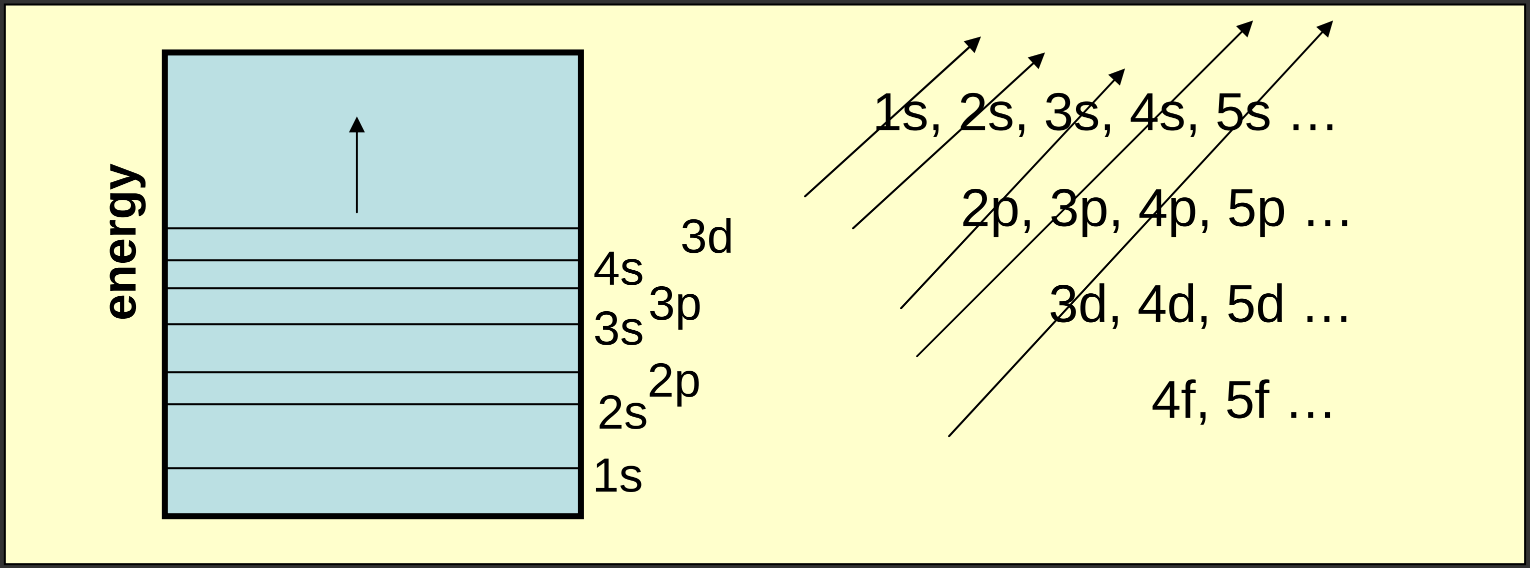
bosons can occupy the same exact quantum state

Rules for Filling of state for multi-electron atom

n, l, m_l, m_s

Spectroscopic notation - s: $l=0$, p: $l=1$, d: $l=2$, f: $l=3$, …

- **No two electrons in same state (Pauli exclusion)**
- **Electrons go into the state with the lowest possible energy (Aufbau)**
- **Within a sublevel, electrons will have their spin unpaired as much as possible (due to spin-spin interaction contribution to energy)**



1s, 2s, 3s, 4s, 5s …

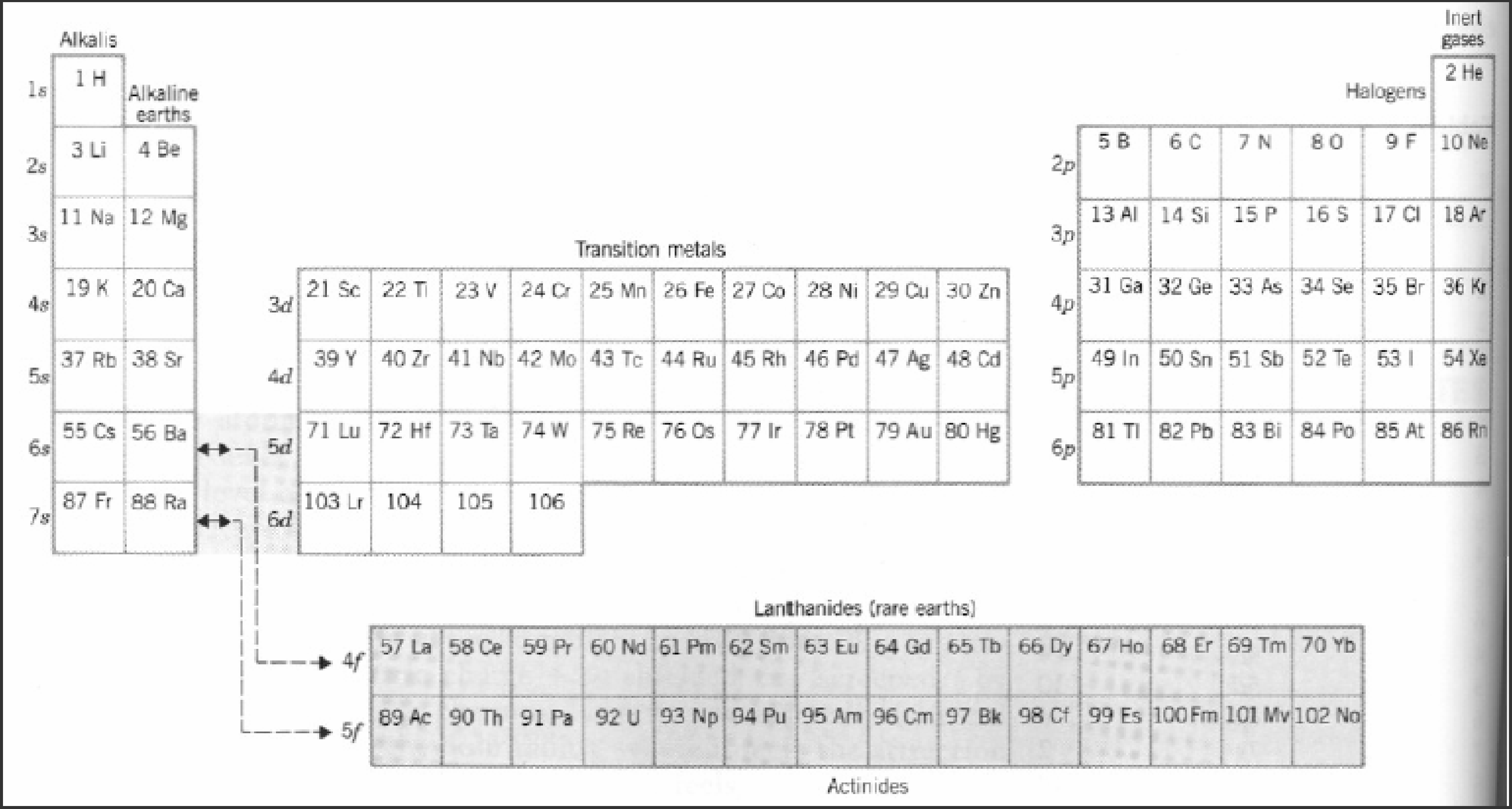
2p, 3p, 4p, 5p …

3d, 4d, 5d …

4f, 5f …

		K shell	L shell				M shell				
Energy level (n)		1	2				3				. . .
Sublevel (ℓ)		s	s	p			s	p			. . .
Z = #e$^-$				$m_\ell=-1$	$m_\ell=0$	$m_\ell=1$					
1	H	↑	—	—	—	—	—	—	—	—	$1s^1$
2	He	↑↓	—	—	—	—	—	—	—	—	$1s^2$
3	Li	↑↓	↑	—	—	—	—	—	—	—	$1s^2 2s^1$
4	Be	↑↓	↑↓	—	—	—	—	—	—	—	$1s^2 2s^2$
5	B	↑↓	↑↓	↑	—	—	—	—	—	—	$1s^2 2s^2 2p^1$
6	C	↑↓	↑↓	↑	↑	—	—	—	—	—	
7	N	↑↓	↑↓	↑	↑	↑	—	—	—	—	
8	O	↑↓	↑↓	↑↓	↑	↑	—	—	—	—	$1s^2 2s^2 2p^4$
9	F	↑↓	↑↓	↑↓	↑↓	↑	—	—	—	—	
10	Ne	↑↓	↑↓	↑↓	↑↓	↑↓	—	—	—	—	
11	Na	↑↓	↑↓	↑↓	↑↓	↑↓	↑	—	—	—	$1s^2 2s^2 2p^6 3s^1$
	⋮				⋮						⋮

Chemistry now “solved”

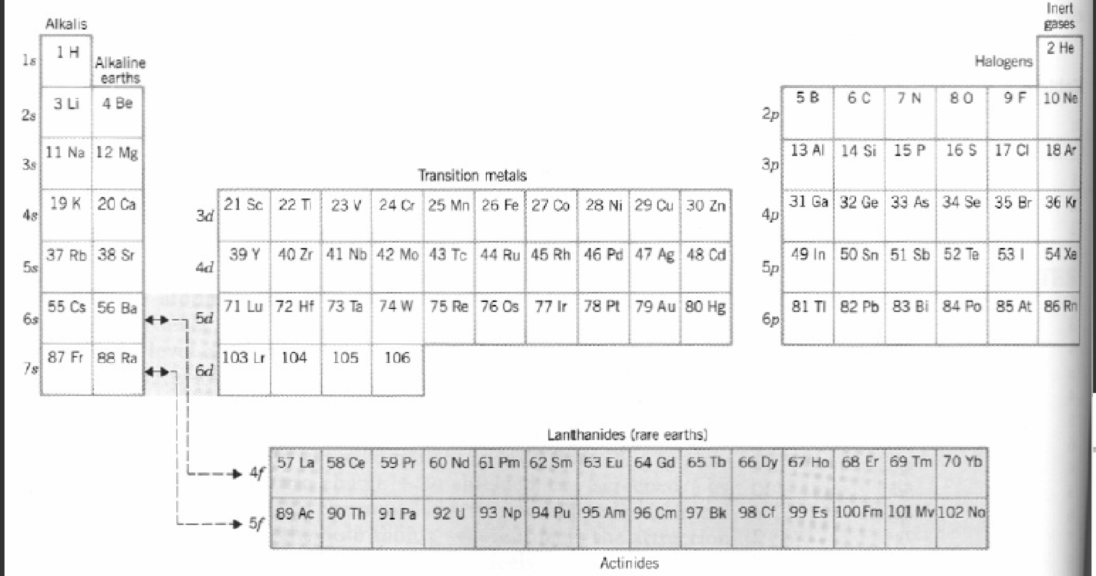


	Alkalis	Alkaline earths		Transition metals															Halogens	Inert gases
1s	1 H																			2 He
2s	3 Li	4 Be												2p	5 B	6 C	7 N	8 O	9 F	10 Ne
3s	11 Na	12 Mg												3p	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4s	19 K	20 Ca	3d	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	4p	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5s	37 Rb	38 Sr	4d	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	5p	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6s	55 Cs	56 Ba	5d	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	6p	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7s	87 Fr	88 Ra	6d	103 Lr	104	105	106													

Lanthanides (rare earths)

4f	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb
5f	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Mv	102 No

Actinides



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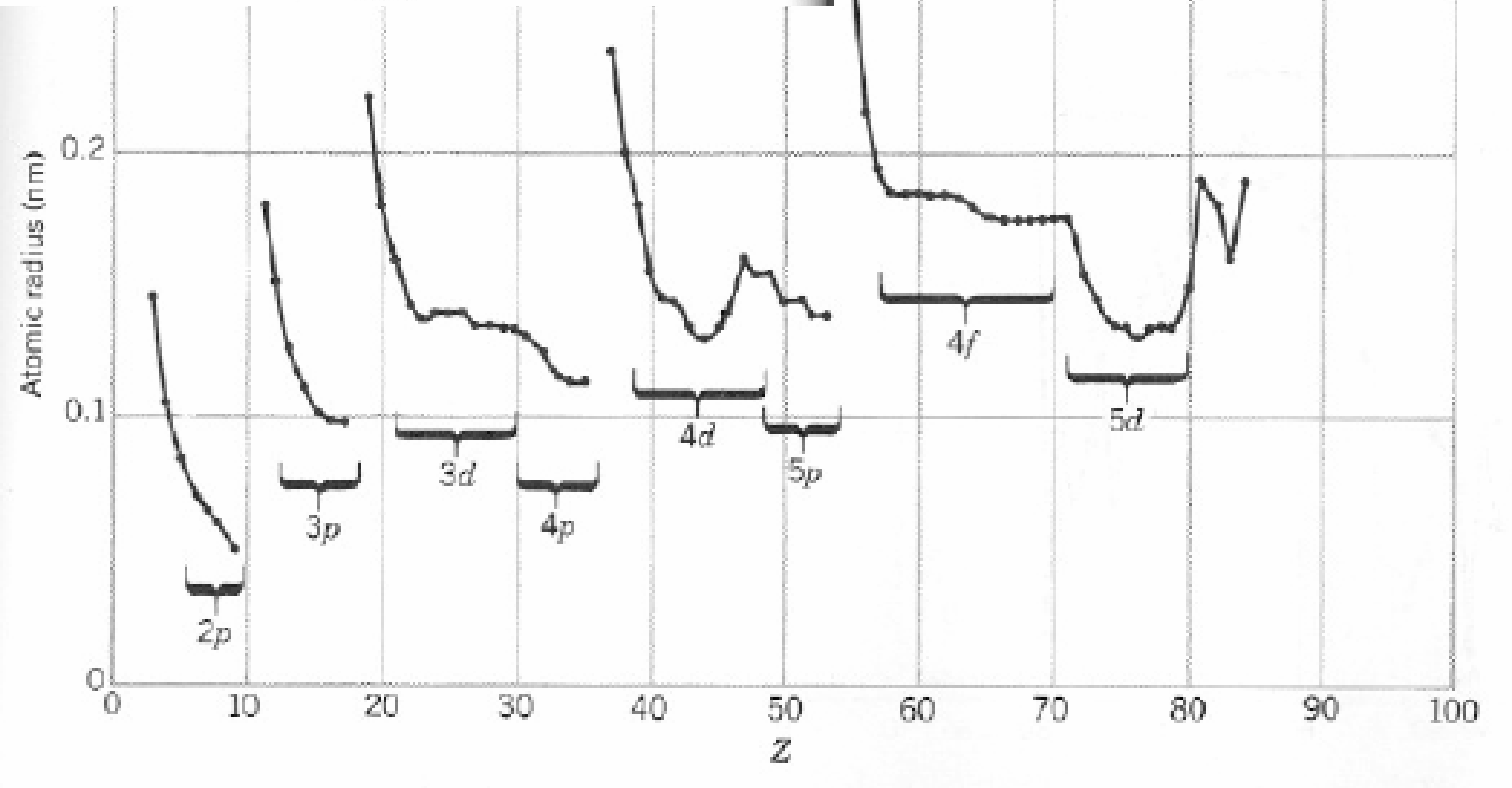

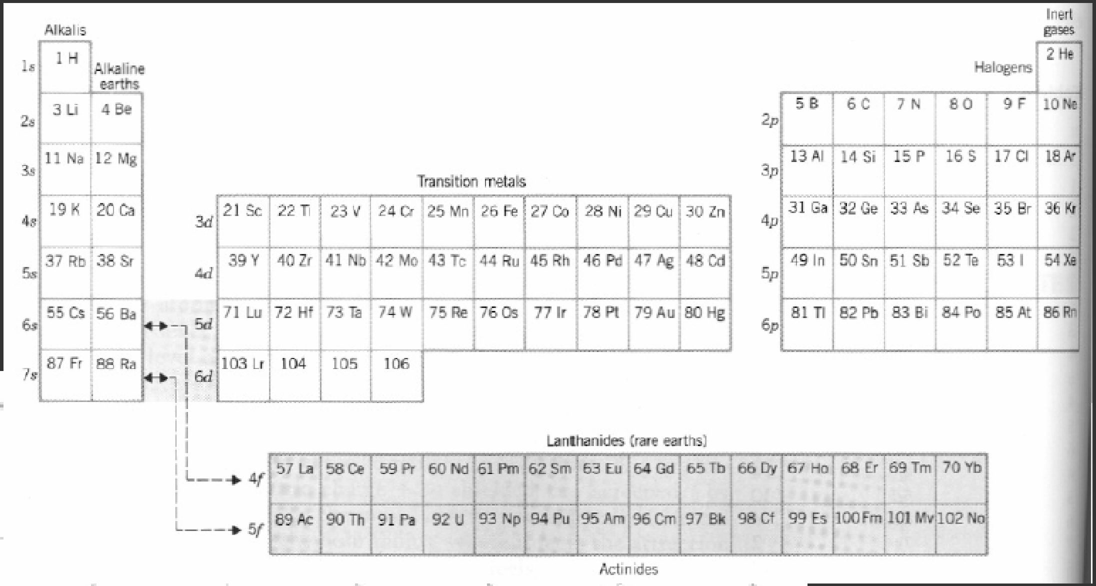

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