Physics 114 - April 20, 2010

- Last class next Tuesday
- Last problem set to hand in This Thursday
- Will give you selected problems/solns in last set of topics — Not for handing in.
- Exam 3 ? Thursday I hope.

Quantum Mechanics

1-d time independent Schrödinger equation

Potential energy function

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U\,\psi(x) = E\,\psi(x)$$

Plug in U and solve for E, ψ

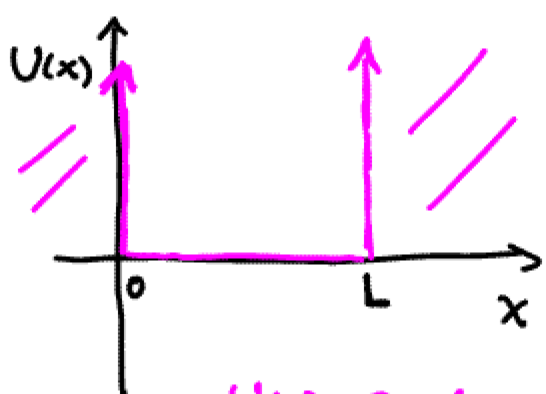
$|\psi|^2 \approx$ probability distribution for particle

$E \equiv$ Allowed energy states for particle

discrete if potential is negative

(force is attractive)

∞ square well potential



$$\frac{d^2\psi(x)}{dx^2} = -\underbrace{\frac{2mE}{\hbar^2}}_{\equiv k^2}\psi(x)$$

$U(x) = 0$ for $0 < x < L$

$U(x) = \infty$ for $x < 0$, $L < x$

Solve eqn → $\psi(x) = A\sin kx + B\cos kx$

Boundary conditions → $\psi(0) = 0$, $\psi(L) = 0$

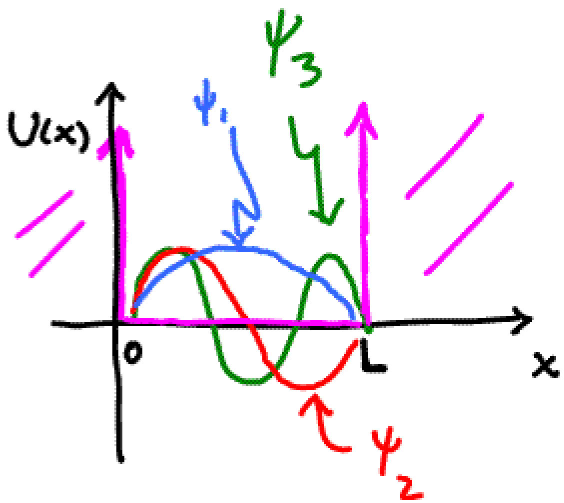
$\psi(x) = A\sin kx$

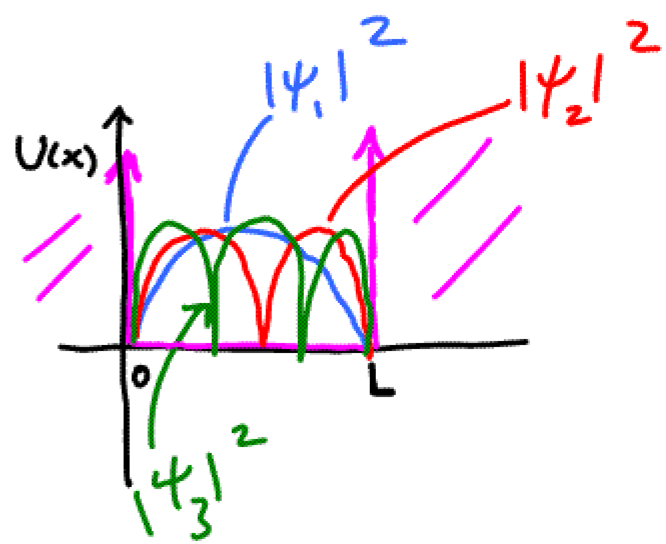
$k_n = \frac{n\pi}{L}$

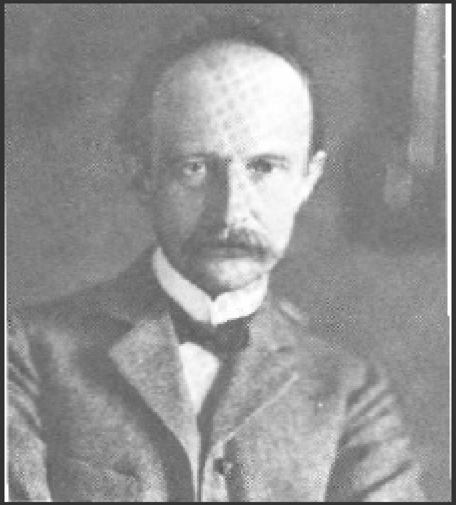
Quantization happens here

$$E_n = \frac{n^2\pi^2\hbar^2}{L^2\, 2m} \qquad n = 1, 2, 3 \ldots$$

$$\psi_n(x) = A\,\mathrm{Sin}\left(\frac{n\pi}{L}x\right) \qquad n = 1, 2, 3 \ldots$$







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

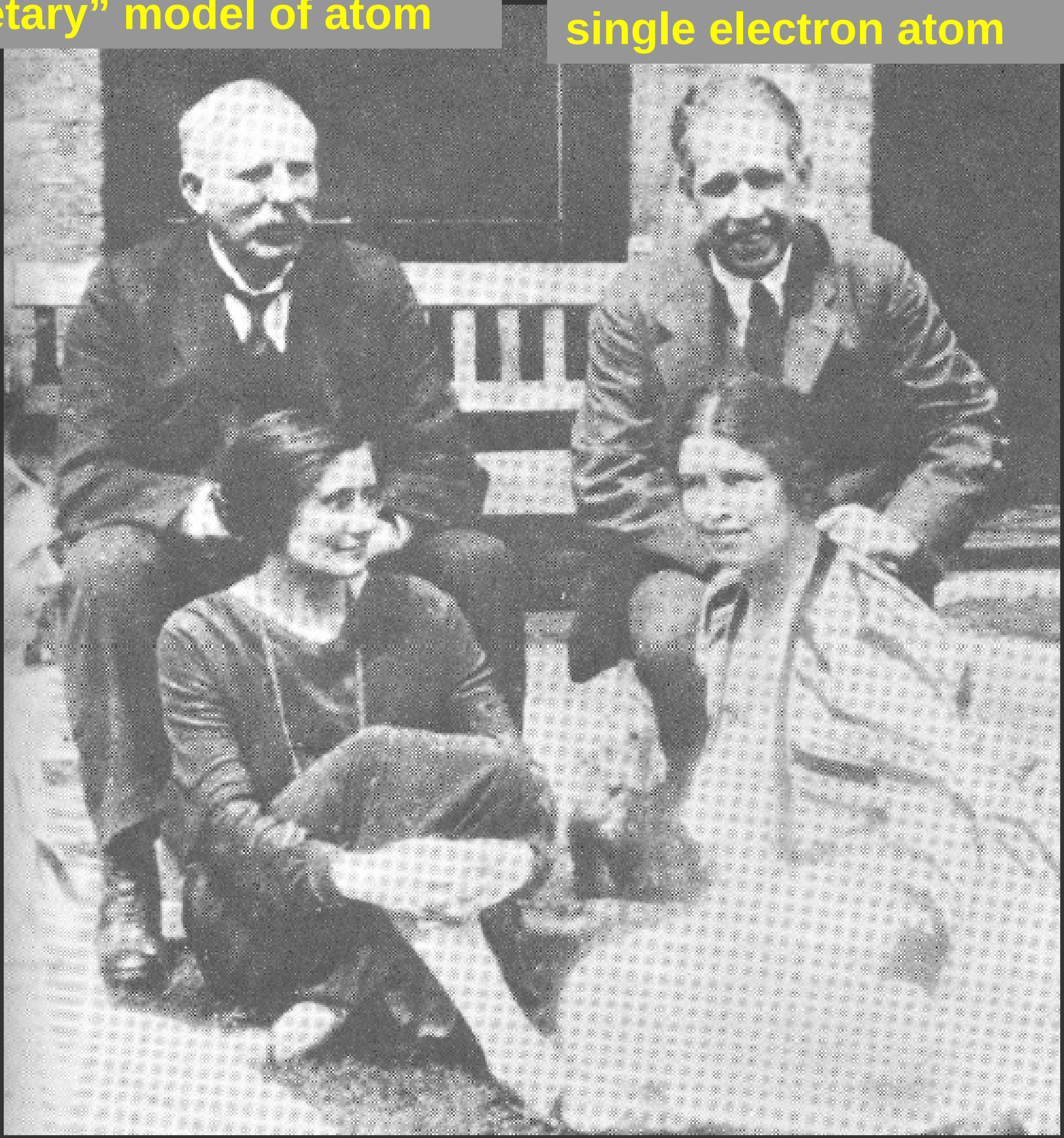
Three of the players

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

$$\underbrace{\frac{-\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2}}_{\text{KE Term}} + \underbrace{V(x)\,\psi(x)}_{\text{PE Term}} = \underbrace{E\,\psi(x)}_{\text{TOT E}}$$

$\psi(x) \equiv$ 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^-

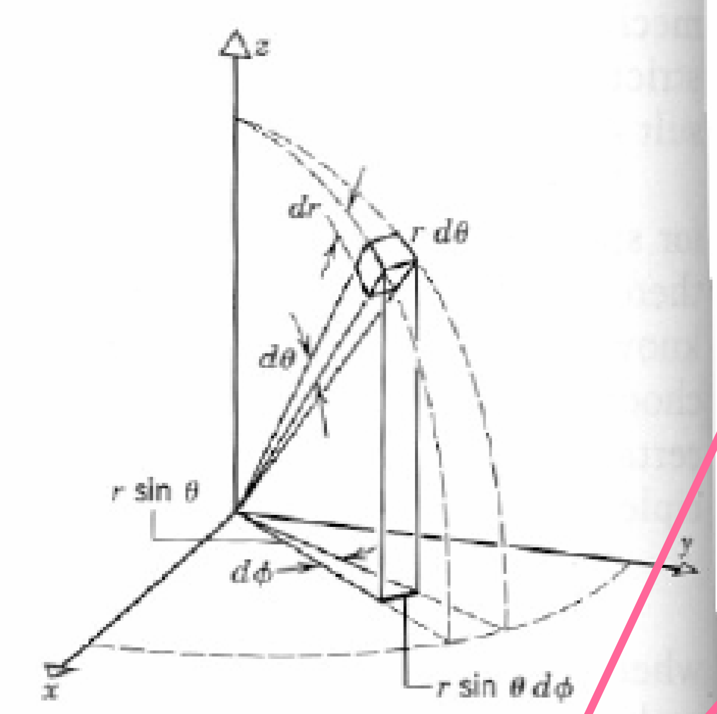
Must generalized to 3d, spherical coordinates

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

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

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

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

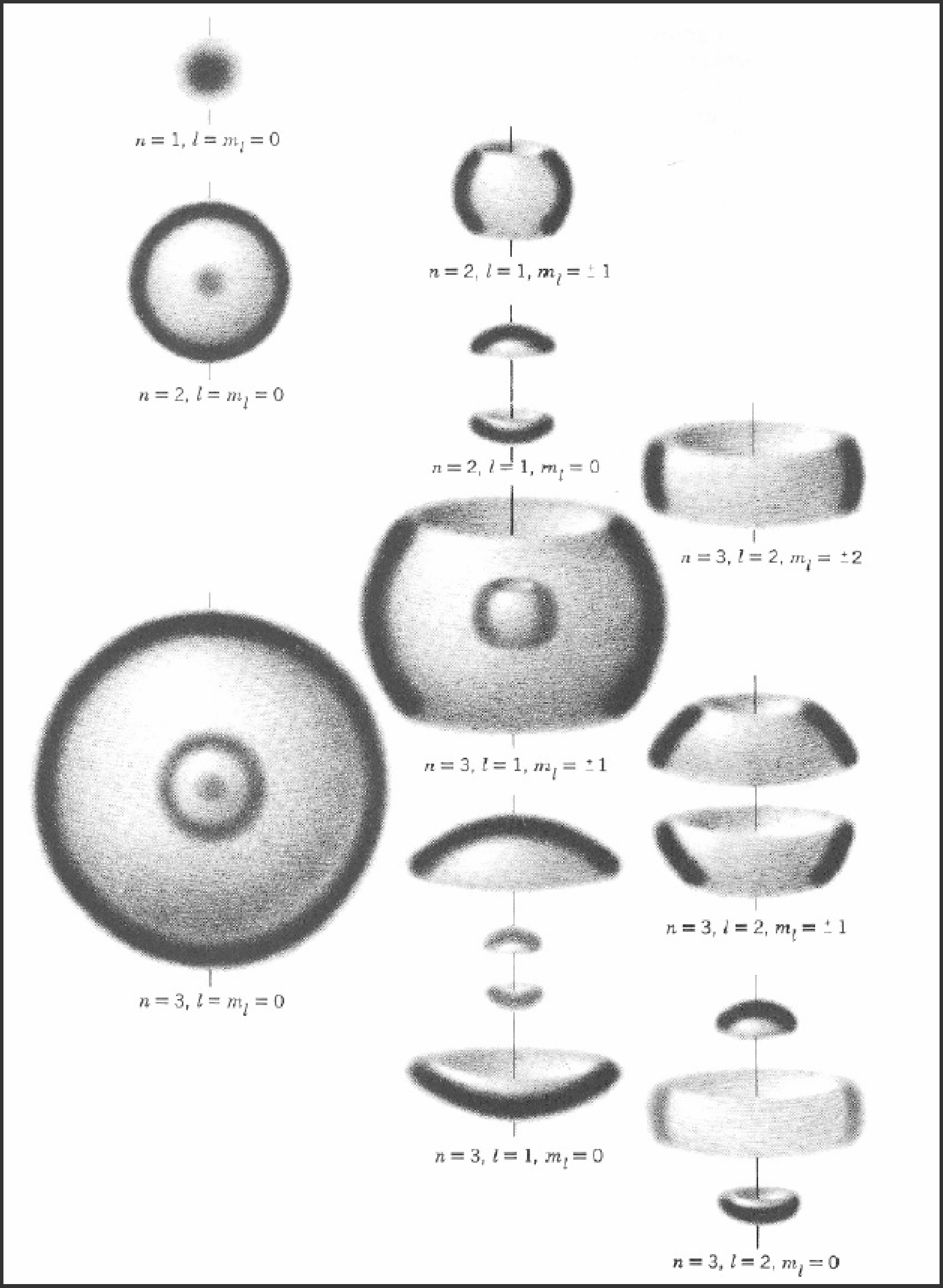
-l, -|l-1|, …, 0, 1, … l-1, l

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

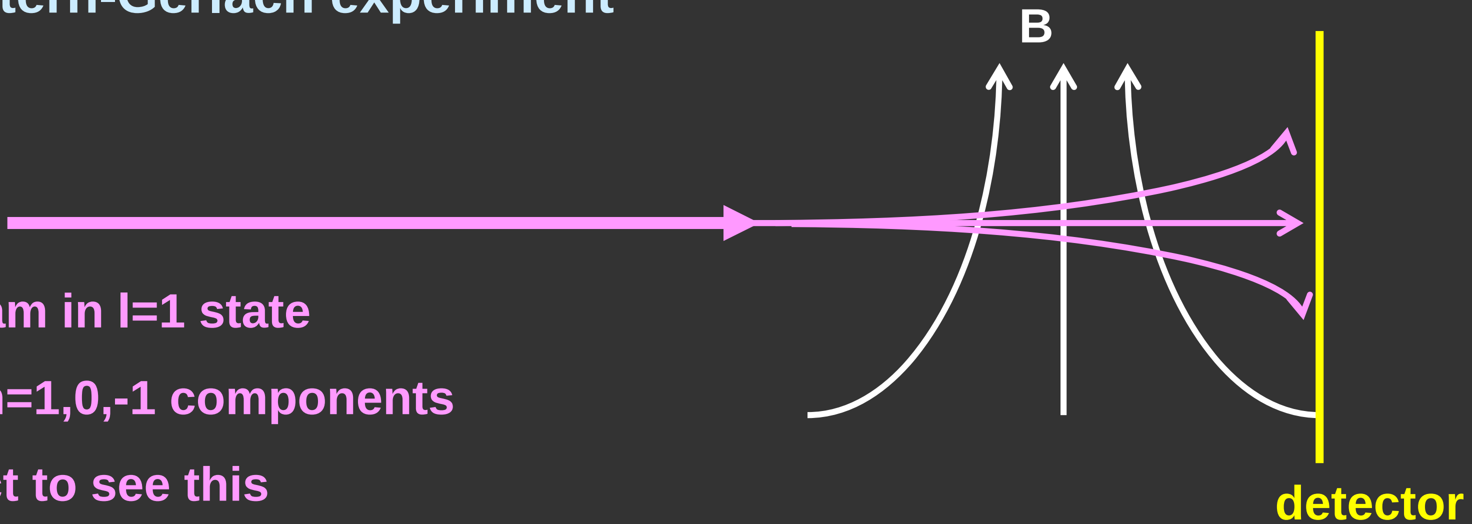
Increasing n adds new radial layers, l=0 give spherical symmetry, l not 0 brings in angular dependence



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

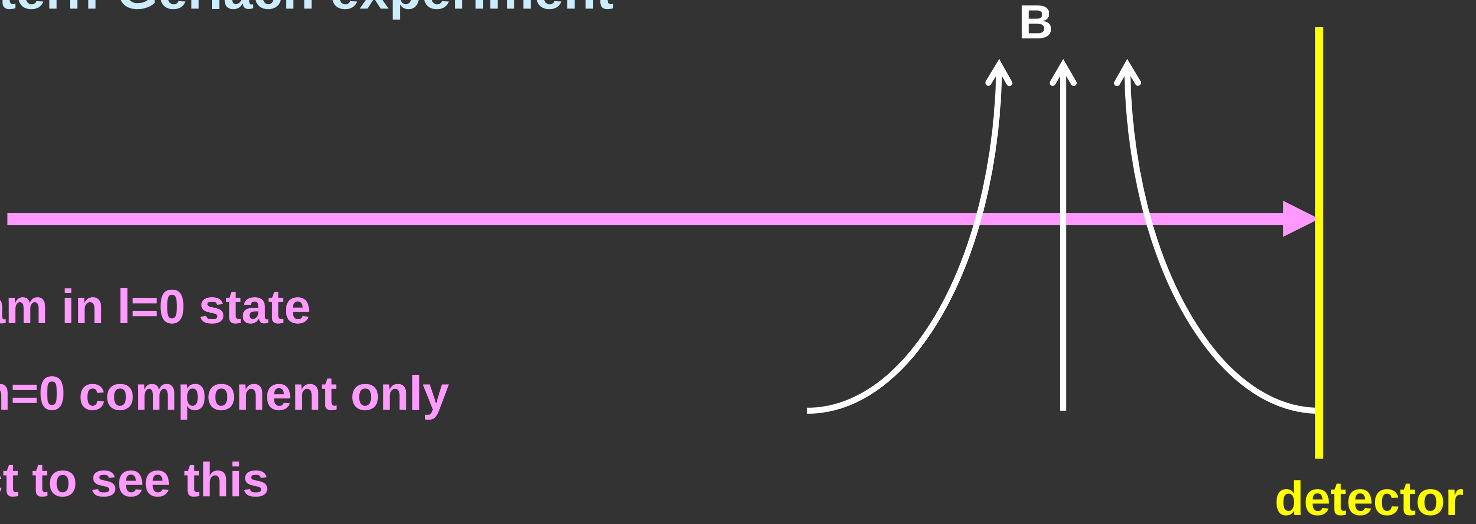
has m=1,0,-1 components

expect to see this

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=0 state

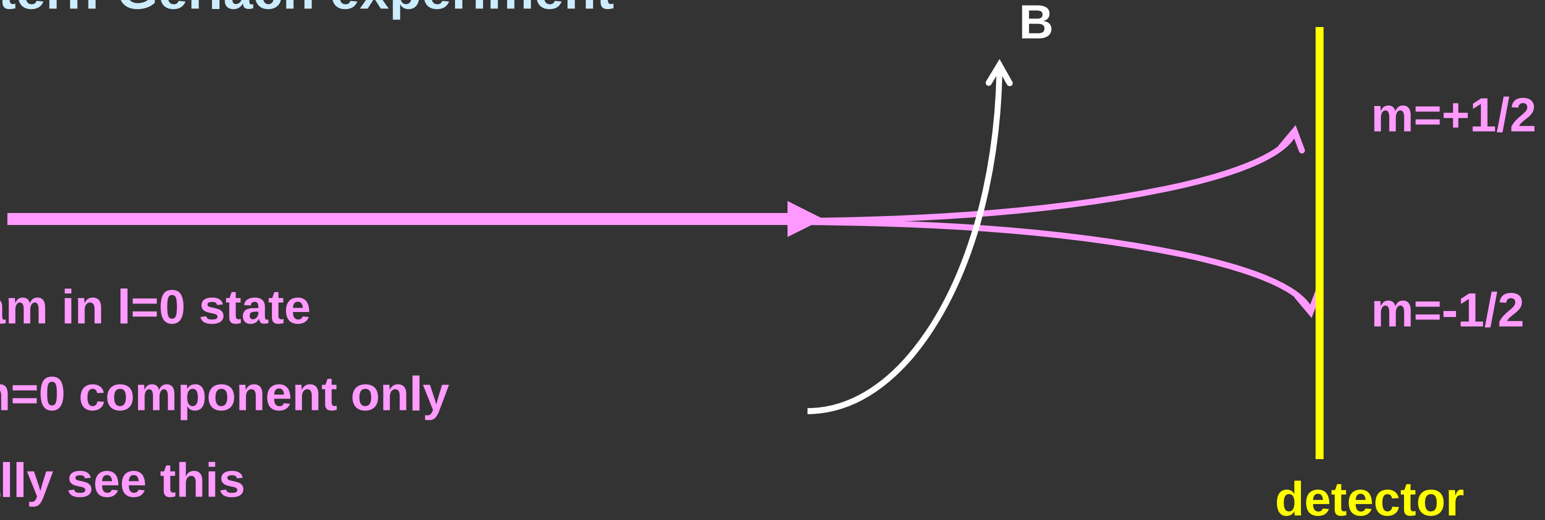
Has m=0 component only

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 …

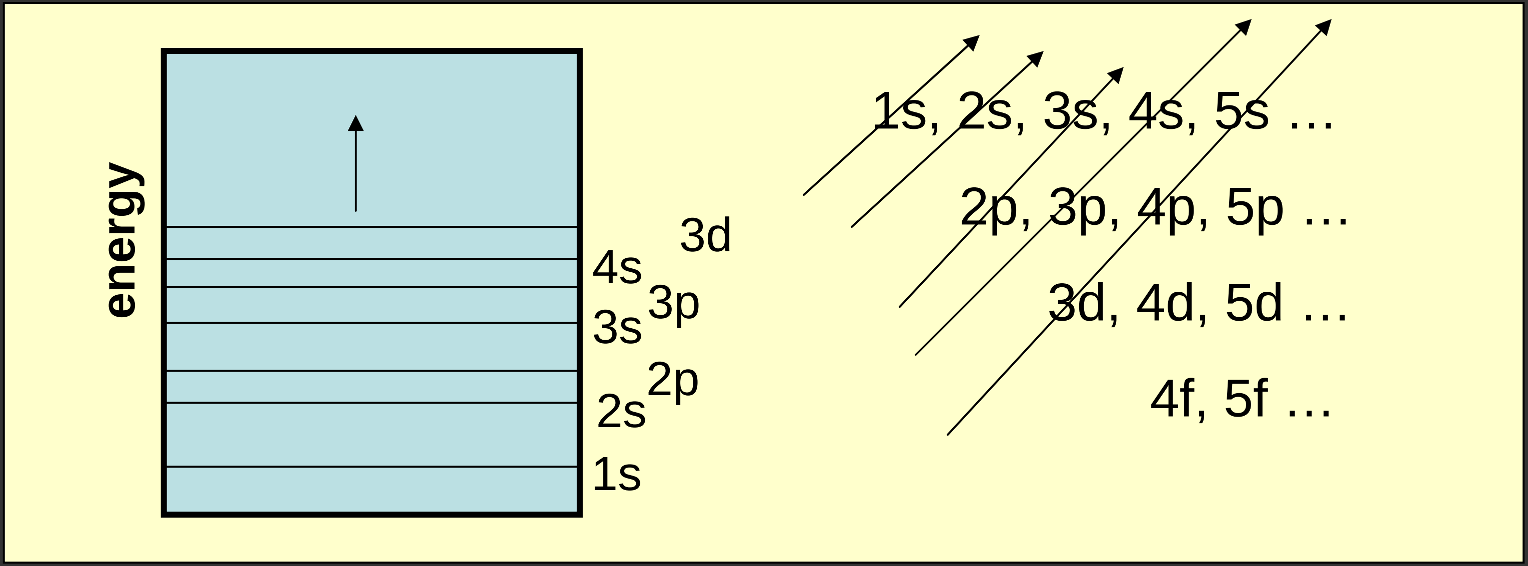
photons (s=1) and pions (s=0) are examples of bosons

bosons can occupy the same exact quantum state

Rules for Filling of state for multi-electron atom
n, l, m_l, m_s

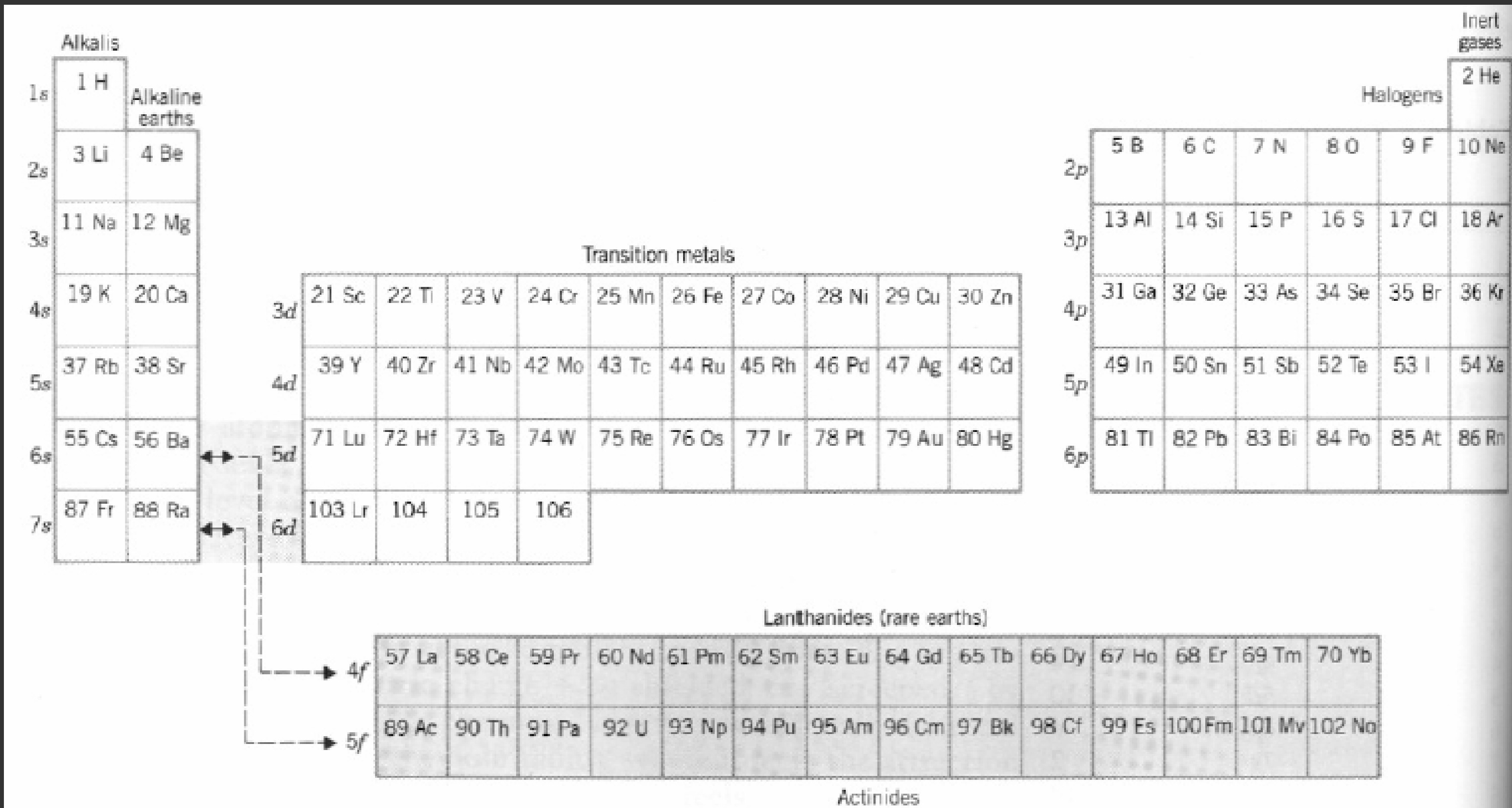
Spectroscopic notation - s: l=0, p: l=1, d: l=2, f: l=3, …

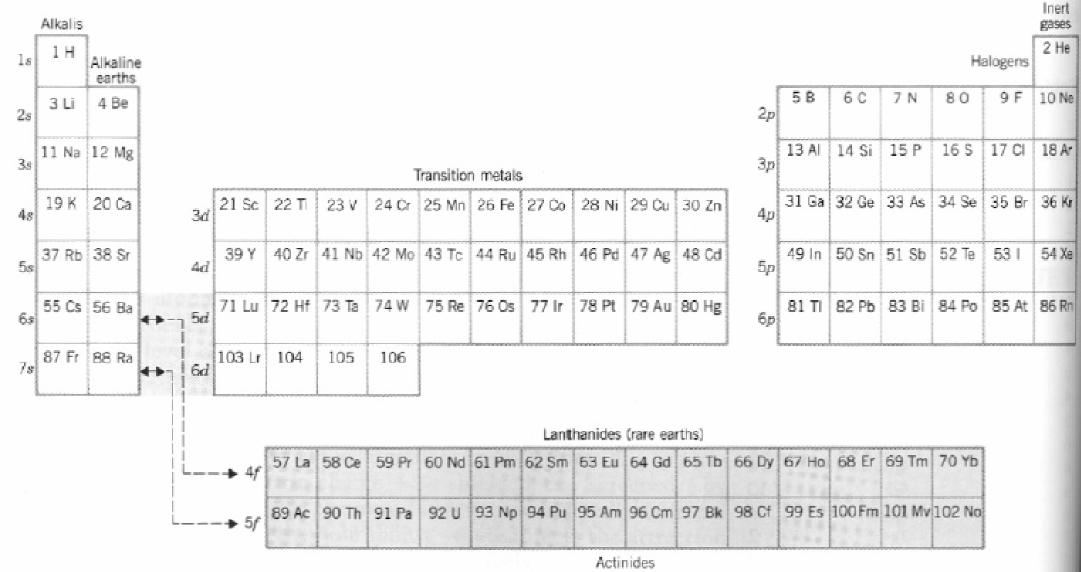
- ➢ No two electrons in same state (Pauli exclusion)
- ➢ Electrons go into the state with the lowest possible energy (Aufbau)
- ➢ Within a sublevel, electrons will have their spin unpaired as much as possible (due to spin-spin interaction contribution to energy)

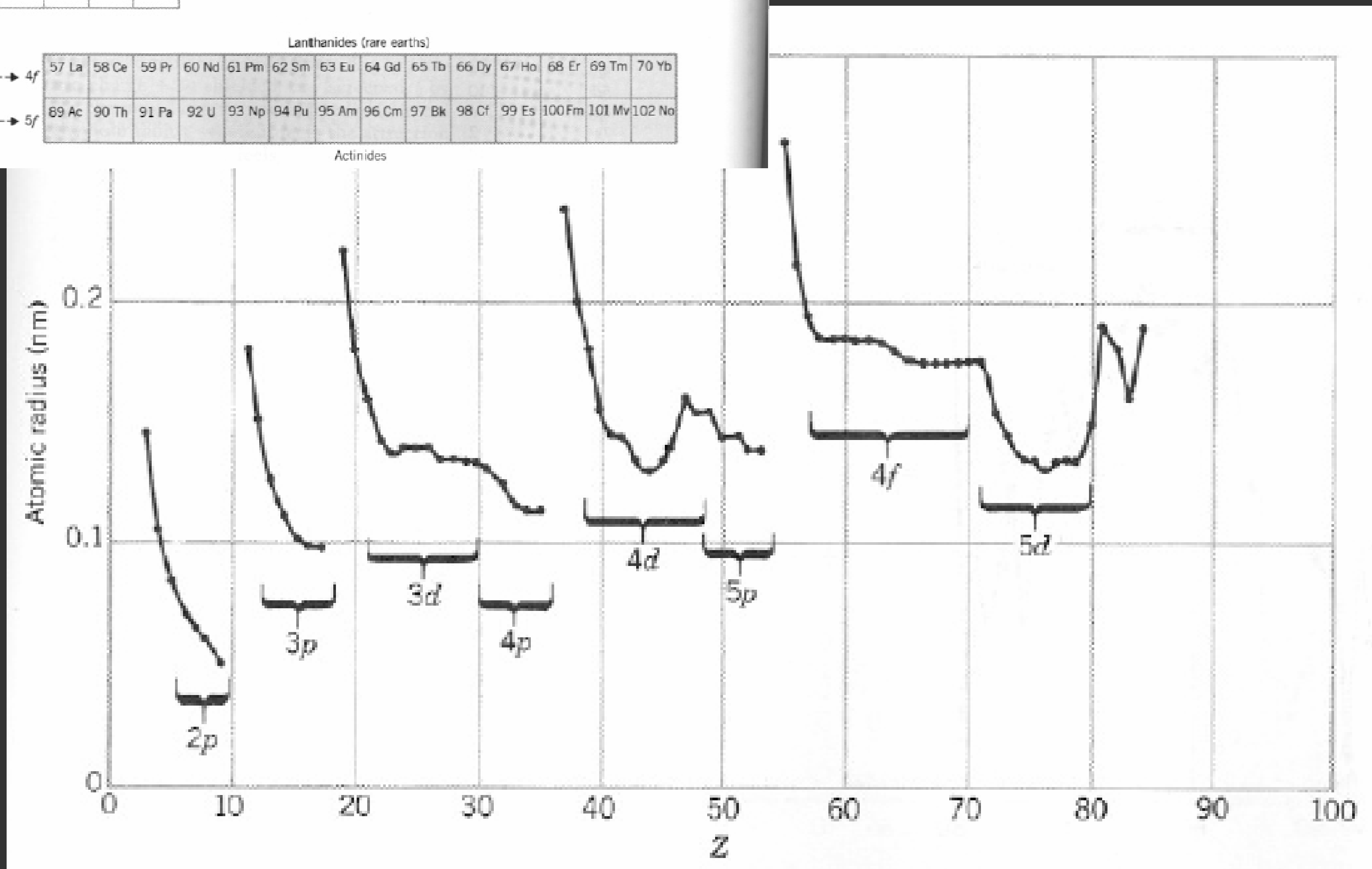


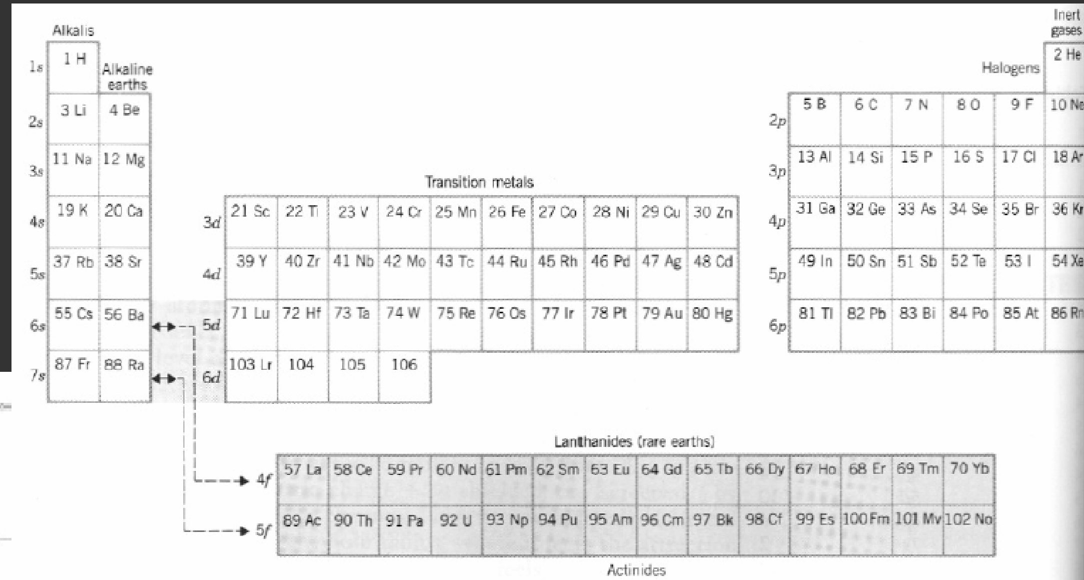
		K shell	L shell				M shell				
	Energy level (n)	1	2				3				. . .
	Sublevel (ℓ)	s	s	p			s	p			. . .
Z = #e^-				$m_\ell=-1$	$m_\ell=0$	$m_\ell=1$					
1	H	↑									$1s^1$
2	He	↑↓									$1s^2$
3	Li	↑↓	↑								$1s^2 2s^1$
4	Be	↑↓	↑↓								$1s^2 2s^2$
5	B	↑↓	↑↓	↑							$1s^2 2s^2 2p^1$
6	C	↑↓	↑↓	↑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

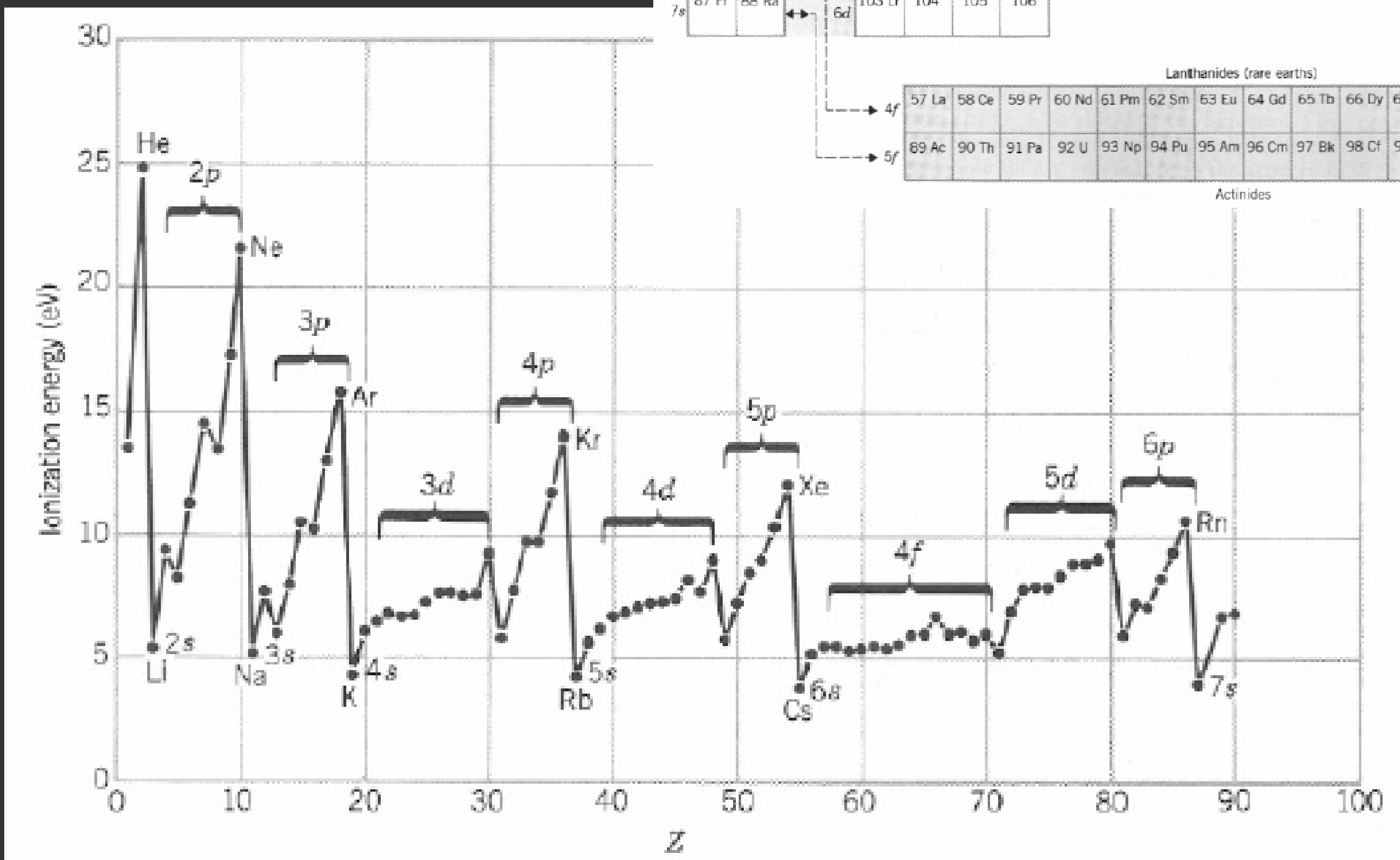
Chemistry now "solved"




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


Atomic radius (nm)
0
0.1
0.2
0
10
20
30
40
50
60
70
80
90
100
Z
2p
3p
3d
4p
4d
5p
4f
5d


Alkalis
Alkaline earths
Inert gases
Halogens
Transition metals
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


Ionization energy (eV)
Z
0
5
10
15
20
25
30
40
50
60
70
80
90
100
He
Ne
Ar
Kr
Xe
Rn
Li
Na
K
Rb
Cs
2s
3s
4s
5s
6s
7s
2p
3p
4p
5p
6p
3d
4d
5d
4f

Magnetic Resonance

Consider a current loop in a $\vec{B}$ field

$$\vec{\tau} = \vec{\mu} \times \vec{B}$$

$$\text{PE of system} = -\vec{\mu} \cdot \vec{B}$$

in QM $\left\{ \begin{array}{l} \text{Spin} \\ \text{Spin component w/ respect to an axis} \end{array} \right\}$ quant.ized

Could be <u>orbital</u> spin

<u>or</u> <u>intrinsic</u> spin

If we define $\vec{B}$ to be along $\hat{z}$

$U \equiv$ energy of interaction of $\vec{\mu}$ w/ $\vec{B}$

$$U = -\mu_z B$$

$$\vec{\mu} = -\frac{1}{2}\frac{e}{m}\vec{L}$$

How Magnetic Moment of e^- in atom depends on $\vec{L}$ (orbital angular momentum)

For e^- in atom $l_z = m_l \hbar$

if $l = 1$ $\quad m_l = -1, 0, +1$

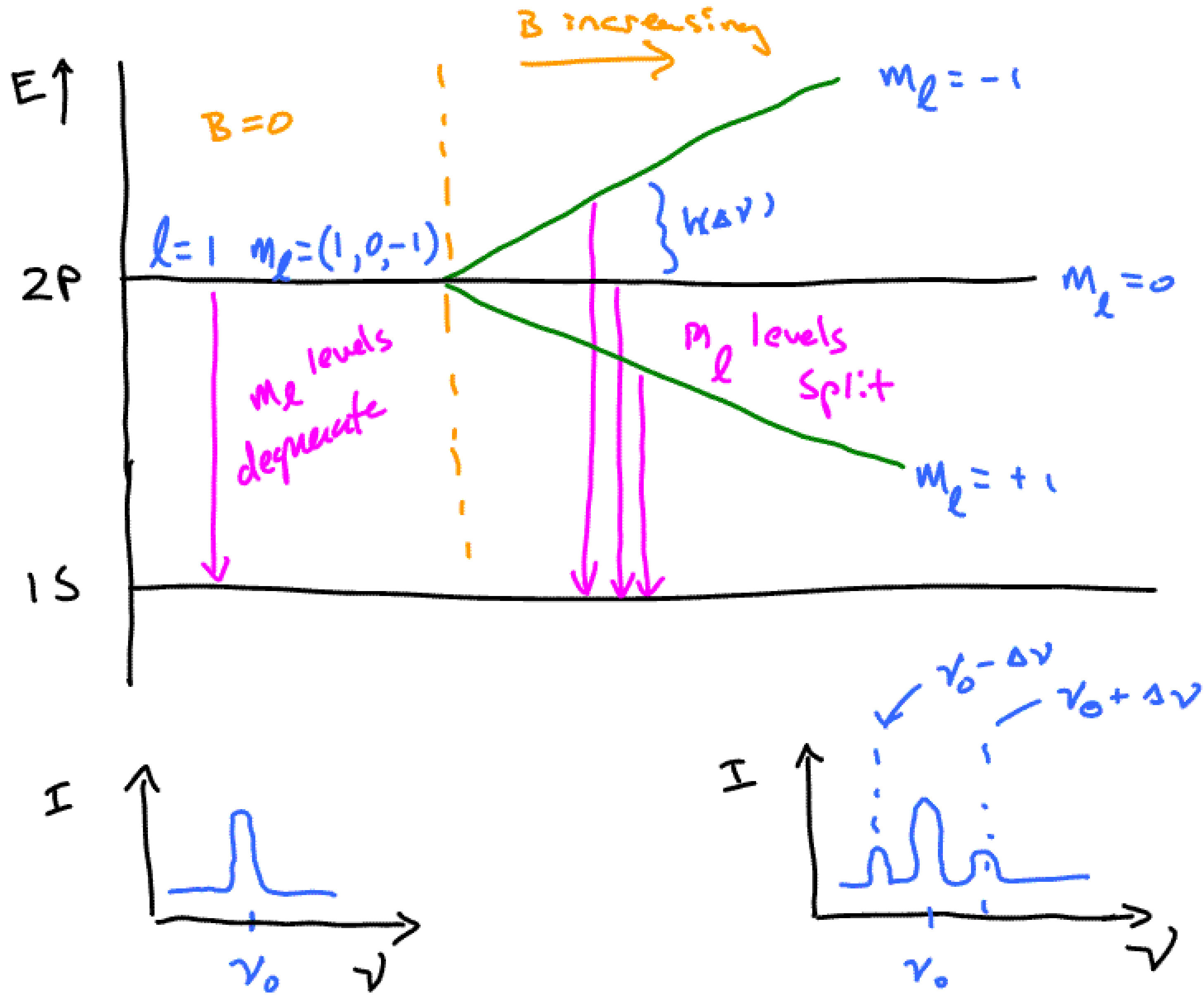
$$l_z = -1\hbar, 0, +\hbar$$

$$\mu_z = \frac{e\hbar}{2m} m_l$$

Bohr magneton $\equiv \mu_B$

Zeeman effect

$U = -\mu_B m_\ell B$ For $\ell = 1$ $m_\ell = -1, 0, +1$



Electron Spin Resonance

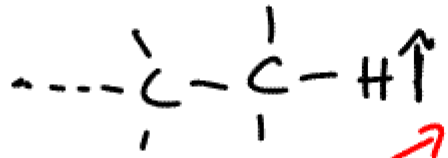
$\vec{B}_{external}$

chemical crud

$\bar{B}_{local}$

unpaired electron

Nuclear Magnetic Resonance



$\vec{B}_{external}$

B_{local}

Scan field . . . or scan frequency