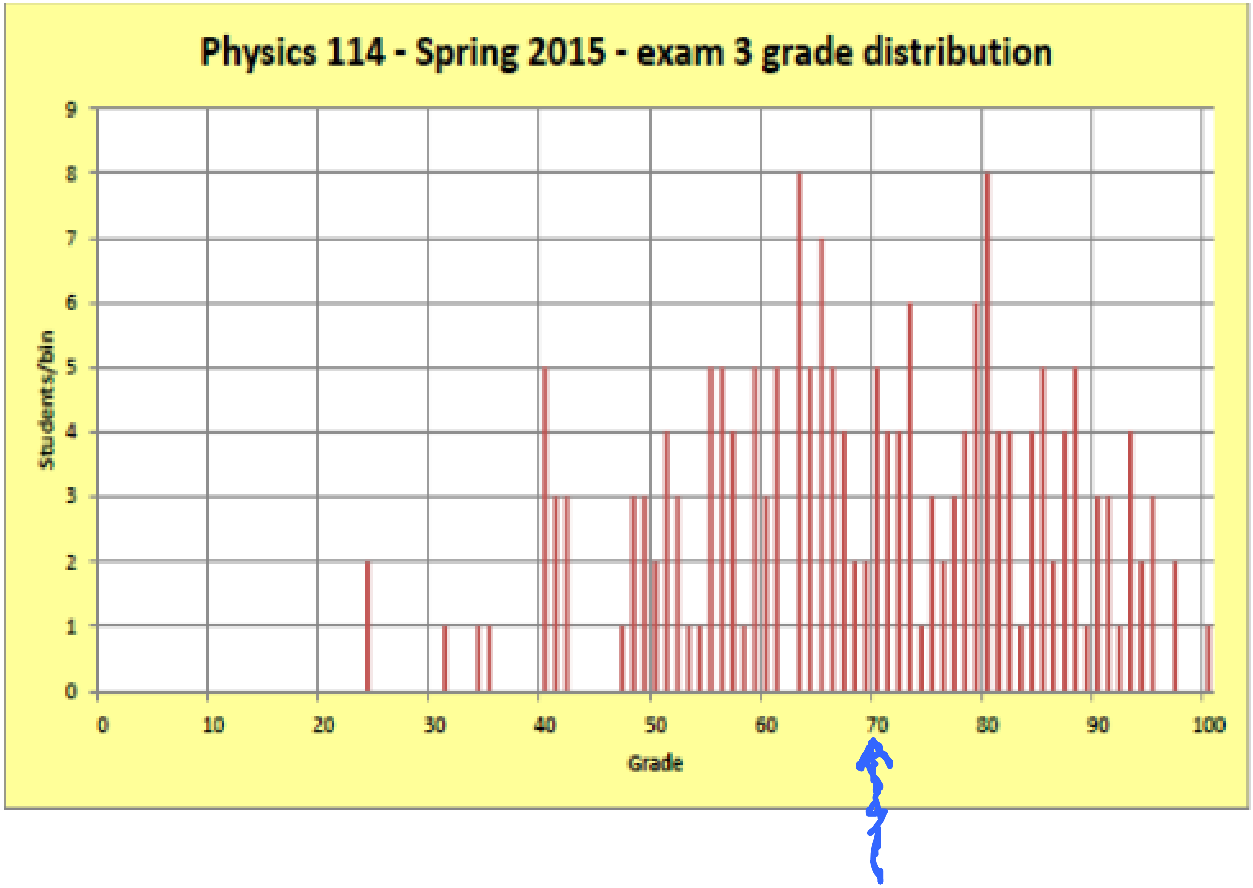
Physics 114 - April 23, 2015

Note Title 4/20/2010

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

Exam 3 – Mean 69, Median 70



Quantum Mechanics

1-d time independent Schrödinger equation

Potential energy function

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

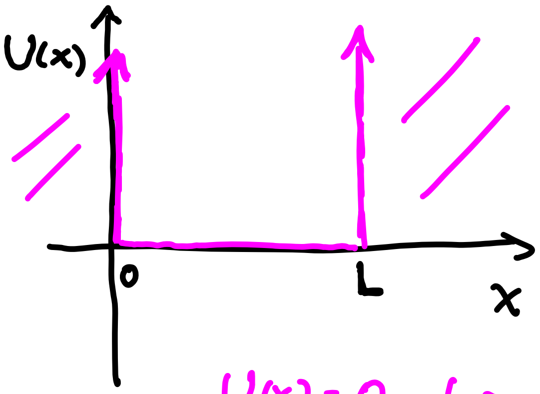
Plug in U and solve for E, ψ

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

$E \equiv$ Allowed energy states for particle

discrete if potential is negative
(force is attractive)

∞ square well potential



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

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

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

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

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

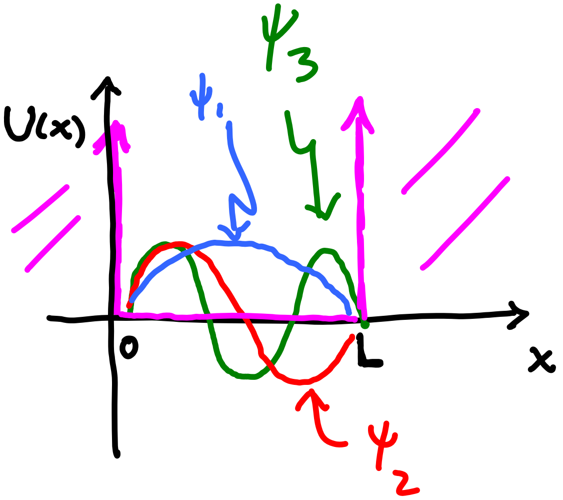
$\psi(x) = A\sin kx$

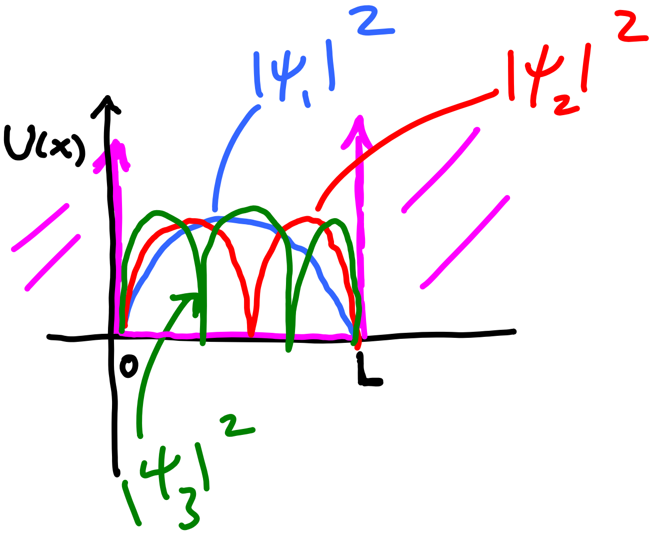
$k_n = \frac{n\pi}{L}$

Quantization happens here

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

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





Attractive Potentials ⇝ discrete
STATES + Energies
Allowed

↓

lead to quantization!

Go to QM and Atoms Slides —

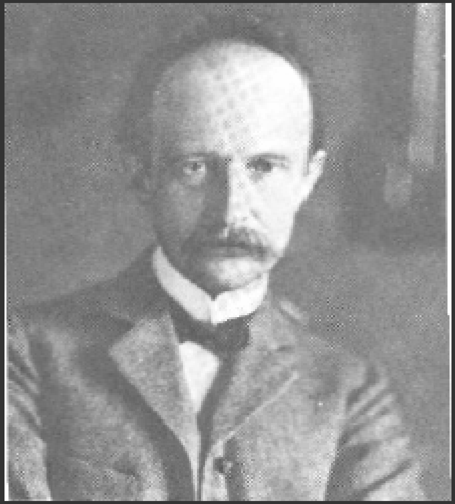
A bit on quantum mechanics and atomic physics

Physics 114

References and photo sources:

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

Three of the players



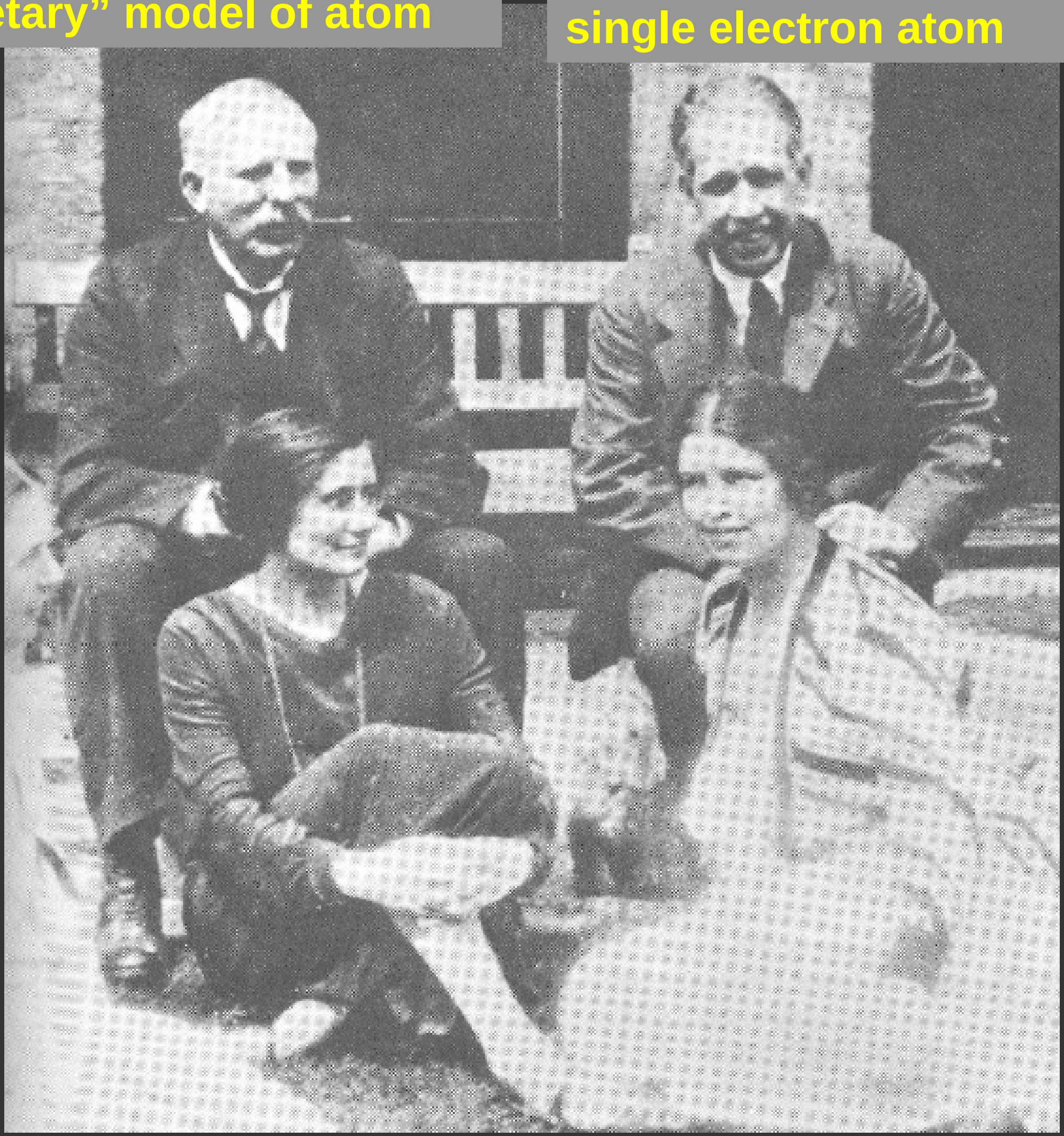
Max Planck (1858-1947) – 1918 Nobel Prize for work on spectral distribution of radiation (blackbody radiation)

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

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

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

What is $\psi(x)$?

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

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

Sub in V as appropriate + solve

for H Atom

p e^-

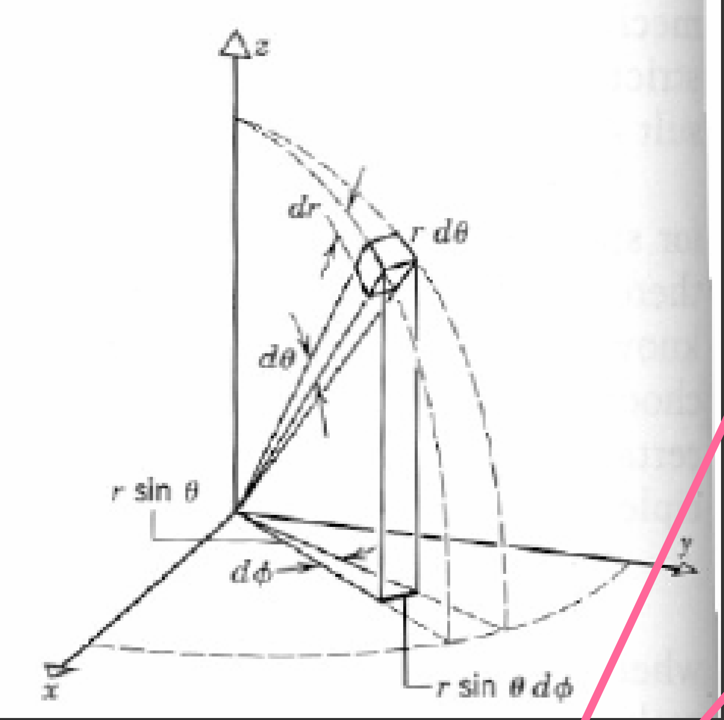
Must generclized to 3d, spherical coordinates

$$V(r) \longrightarrow \frac{1}{4\pi\varepsilon_0}\frac{|q|^2}{r^2}$$ + Solve

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

$$+ \frac{1}{4\pi\varepsilon_0}\frac{|e|^2}{r^2}\psi(r) = E\,\psi(r)$$

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

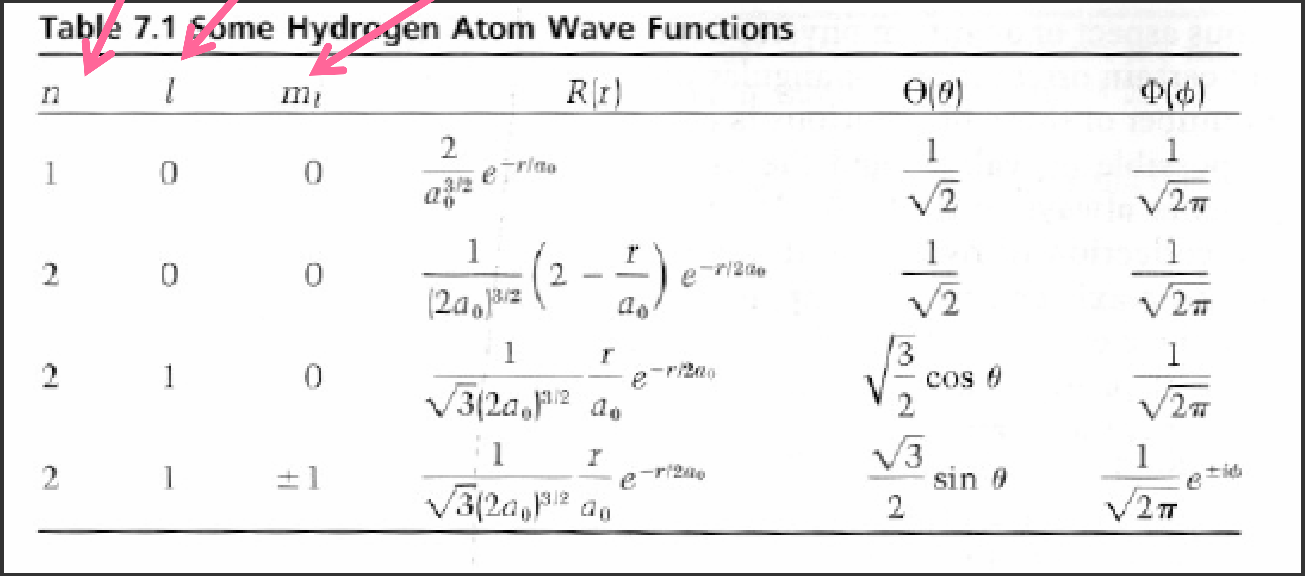
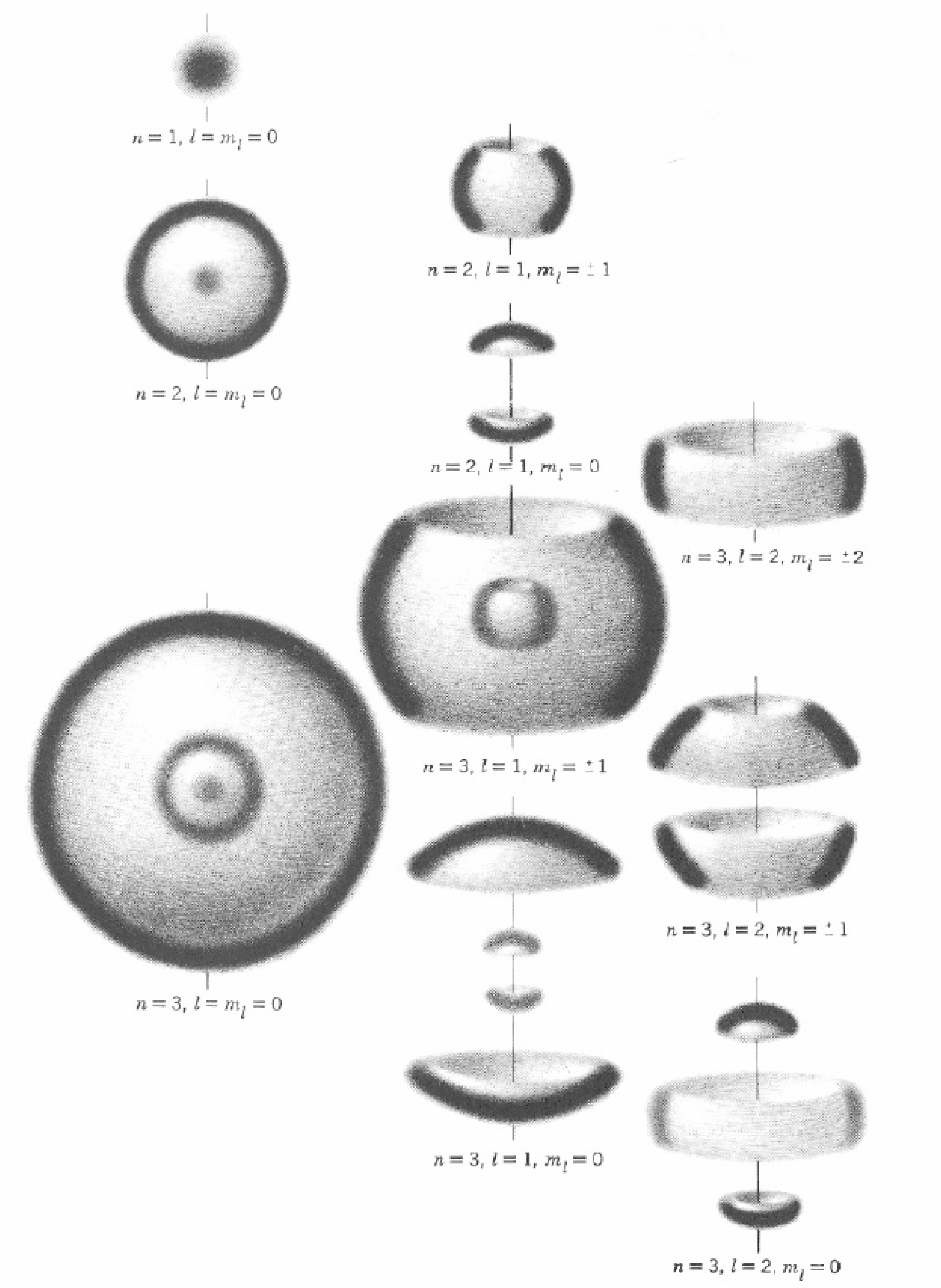


Table 7.1 Some Hydrogen Atom Wave Functions

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

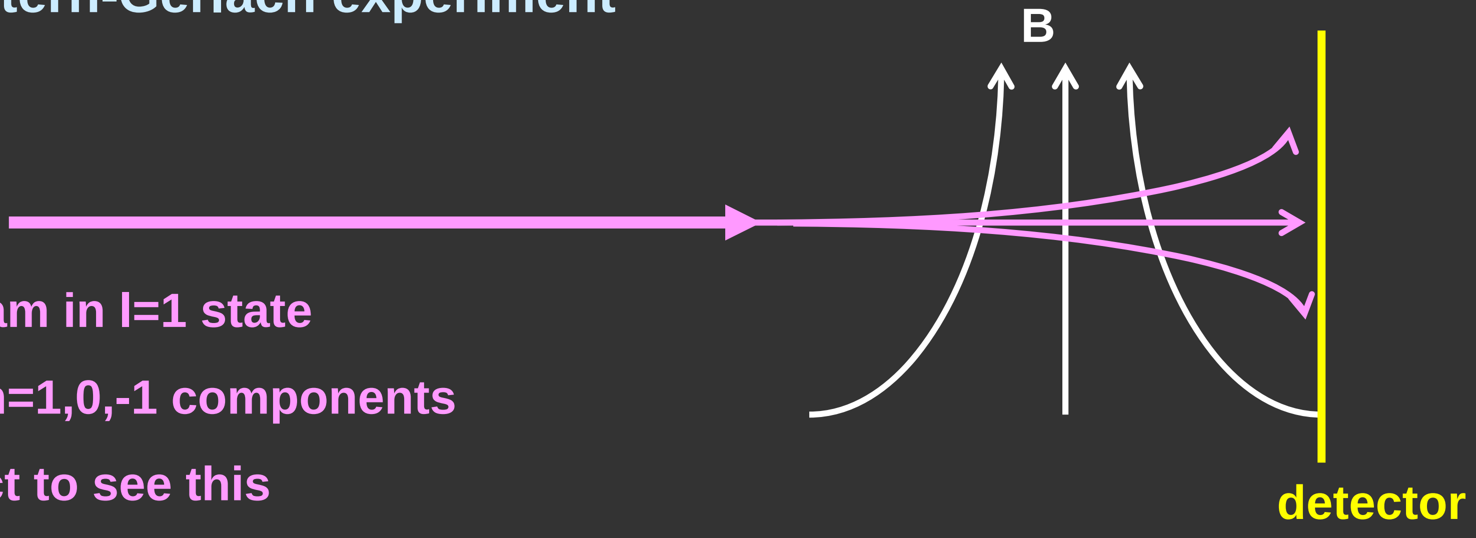
Increasing n adds new radial layers, l=0 give spherical symmetry, l not 0 brings in angular dependence



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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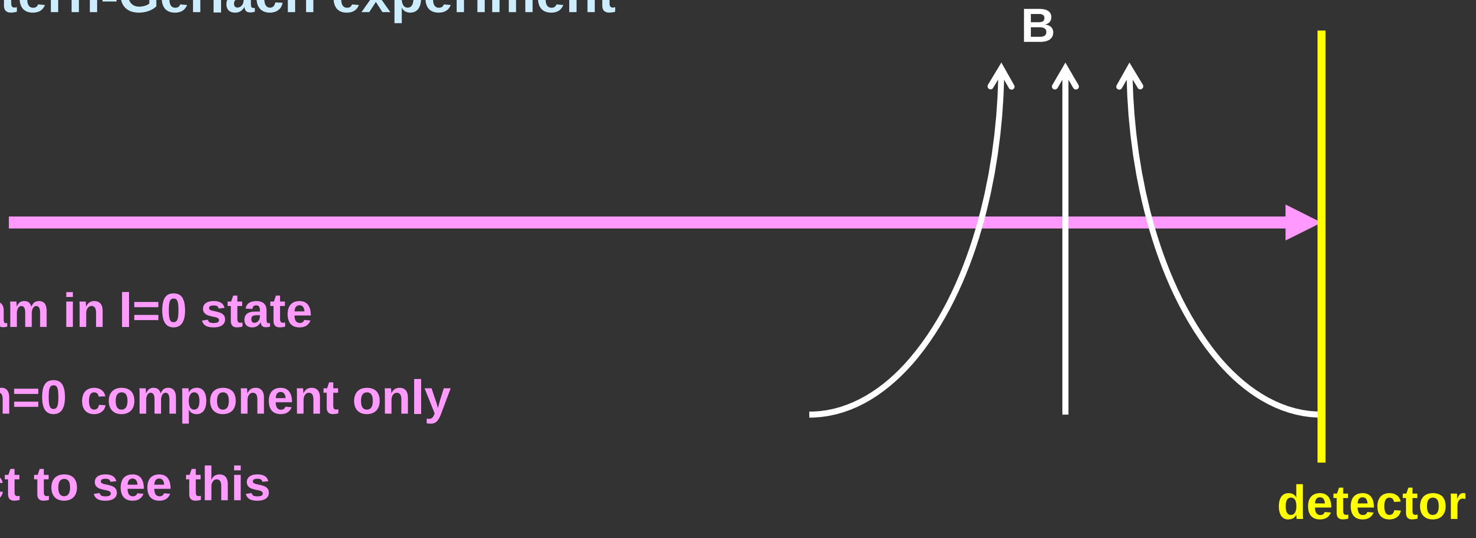


e- beam in l=0 state

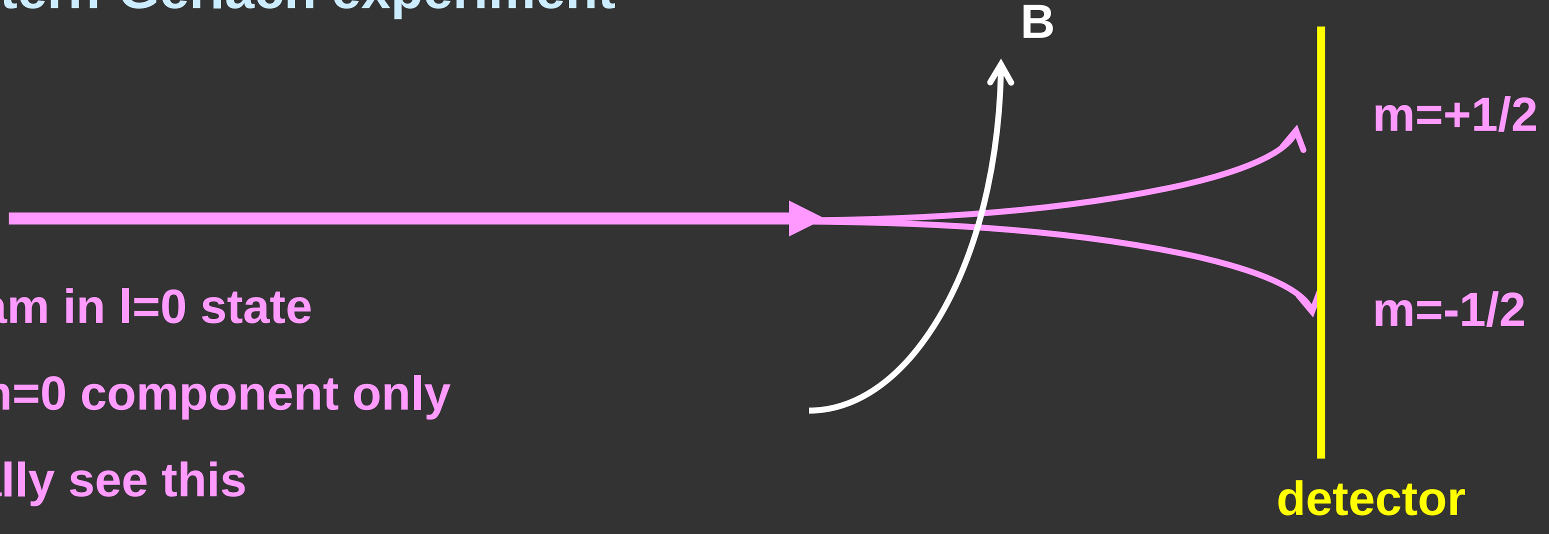
Has m=0 component only

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 …

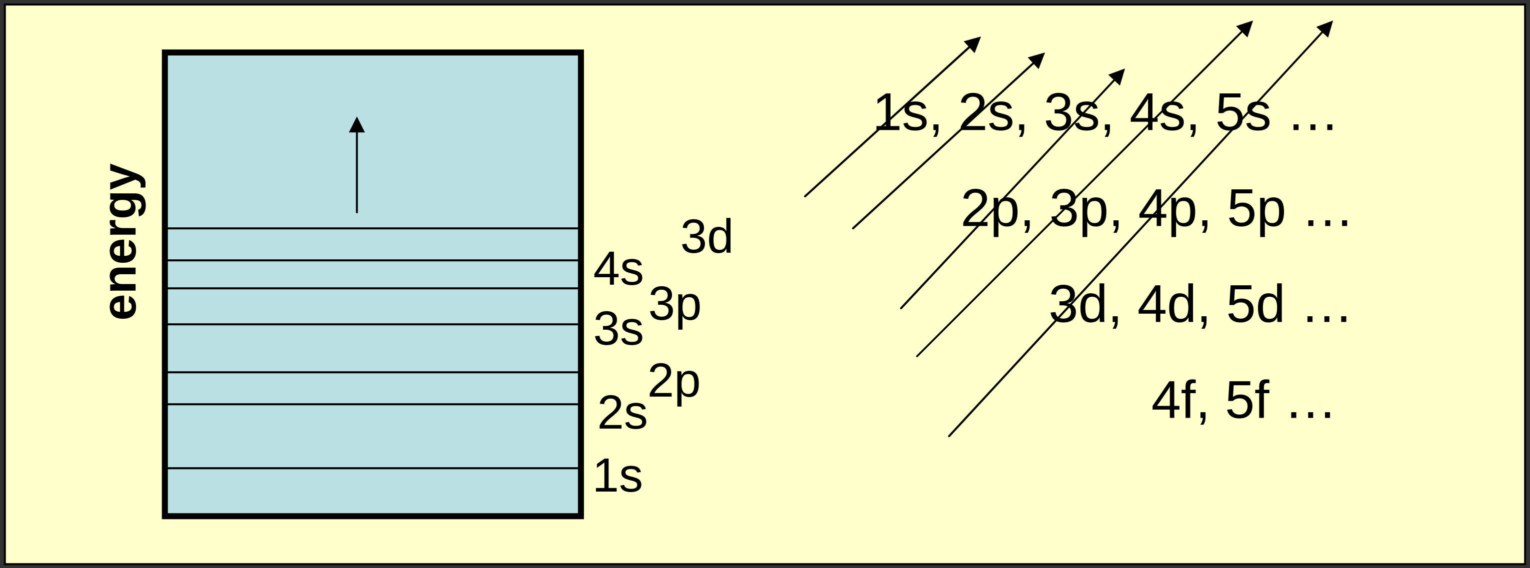
photons (s=1) and pions (s=0) are examples of bosons

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 …

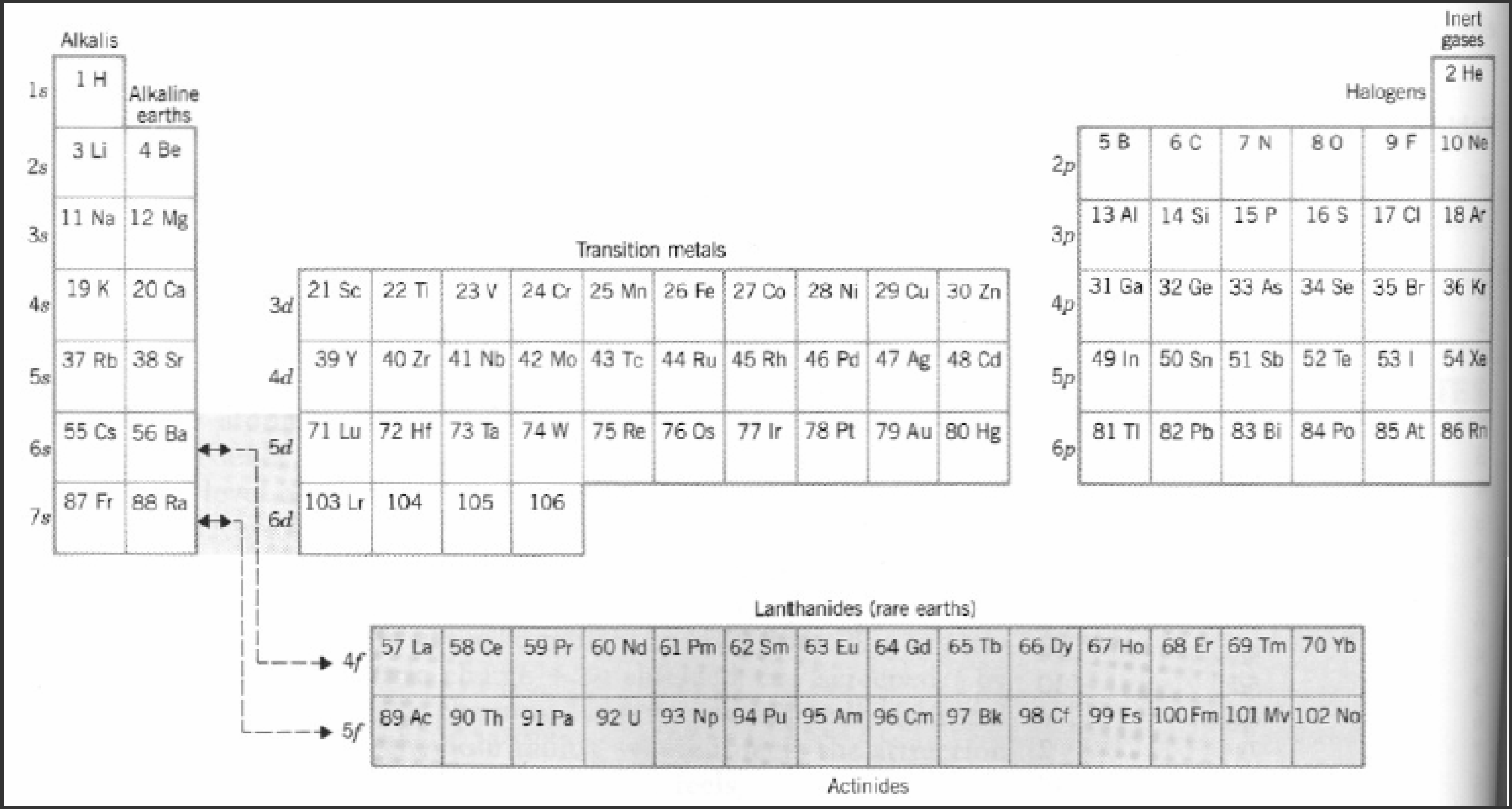
2p, 3p, 4p, 5p …

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”

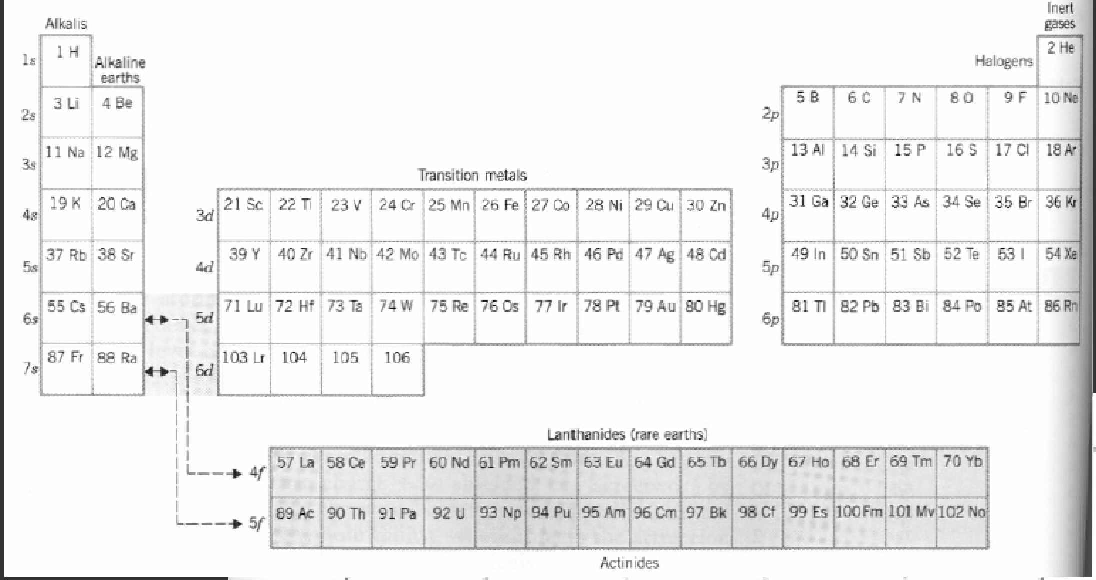


	Alkalis	Alkaline earths		Transition metals															Halogens	Inert gases
1s	1 H																			2 He
2s	3 Li	4 Be												2p	5 B	6 C	7 N	8 O	9 F	10 Ne
3s	11 Na	12 Mg												3p	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4s	19 K	20 Ca	3d	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	4p	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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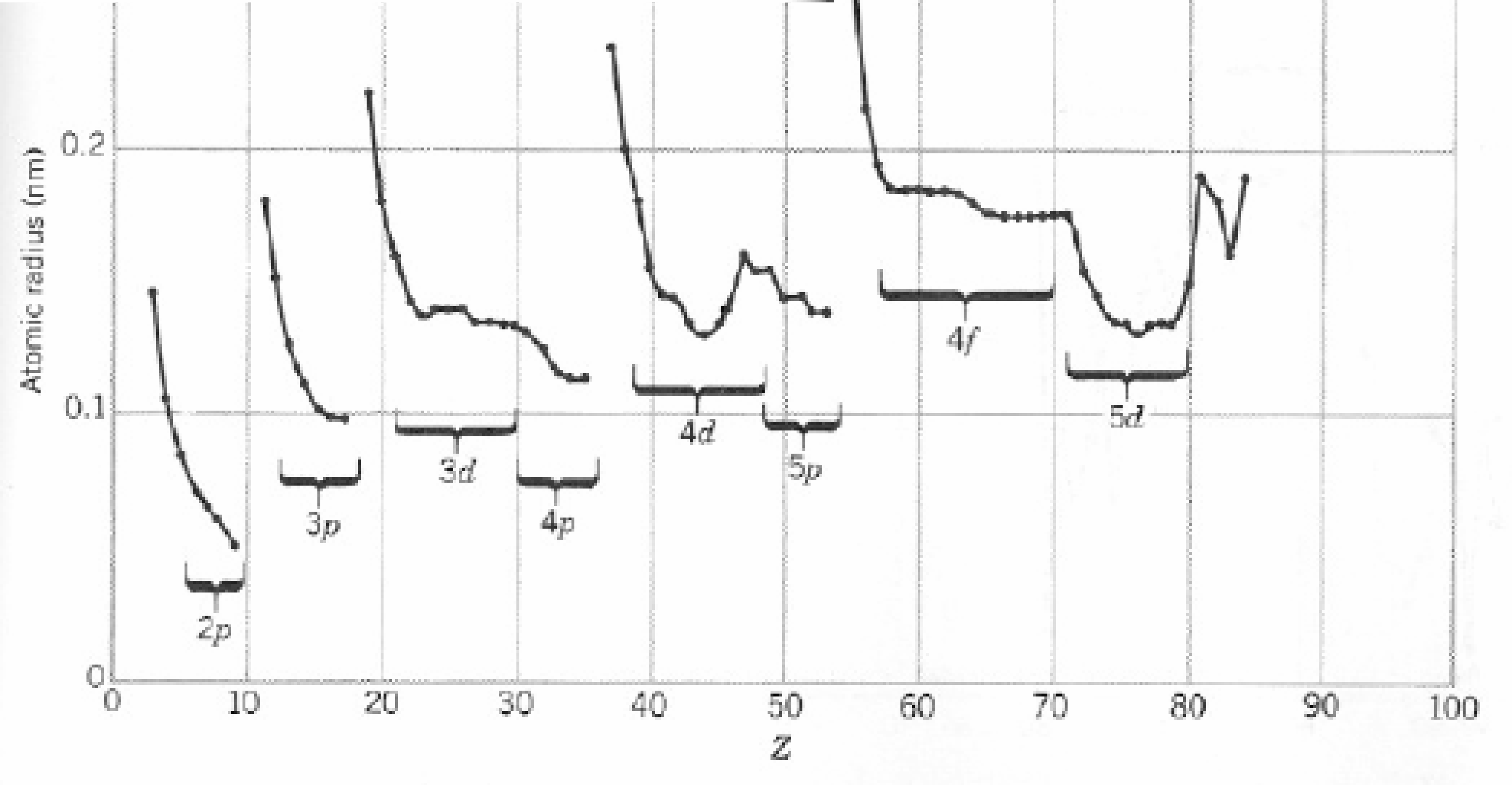

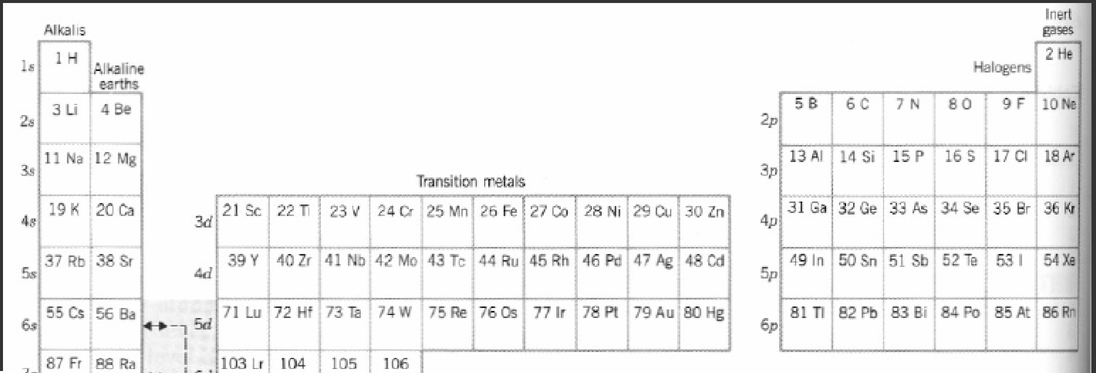

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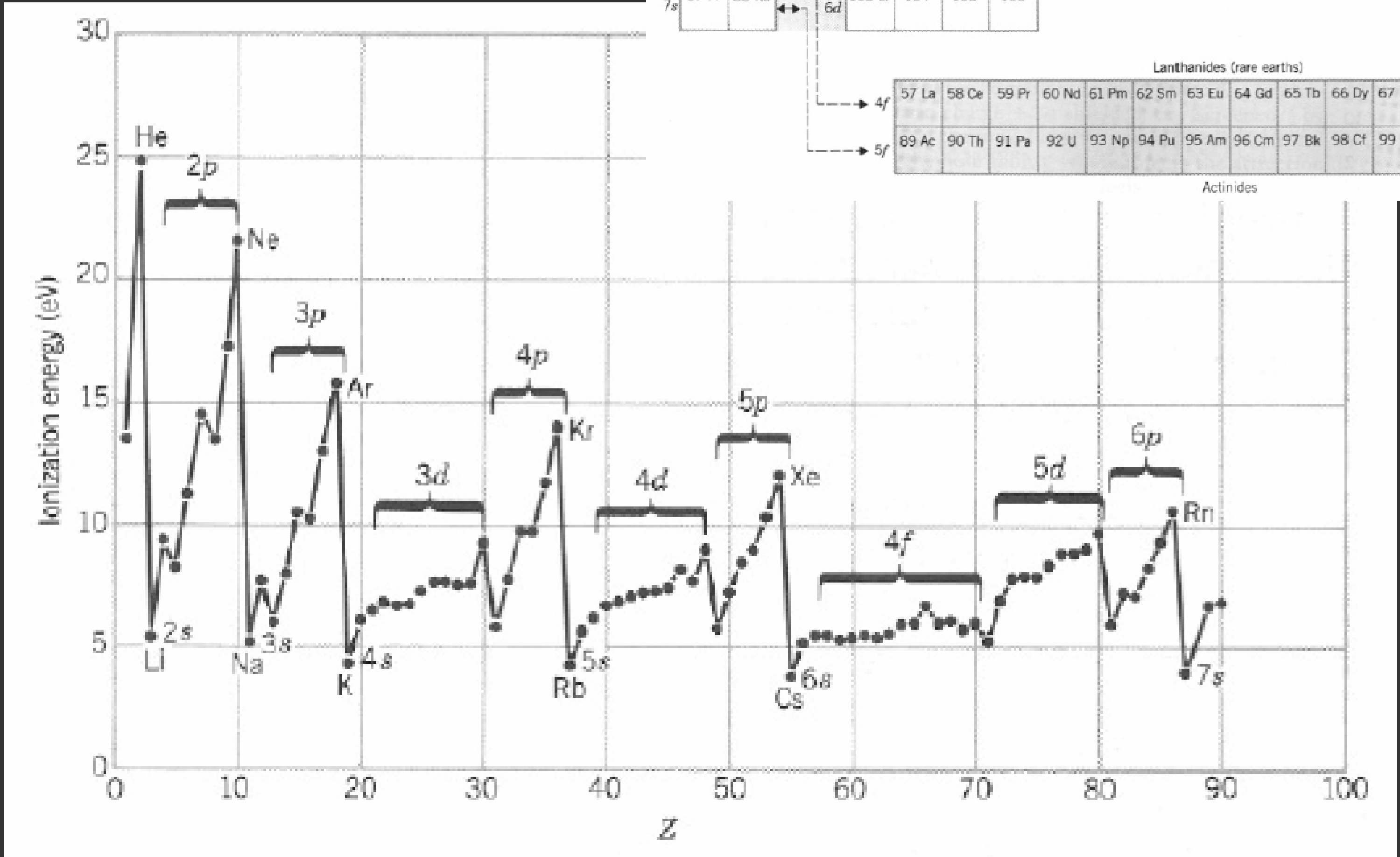
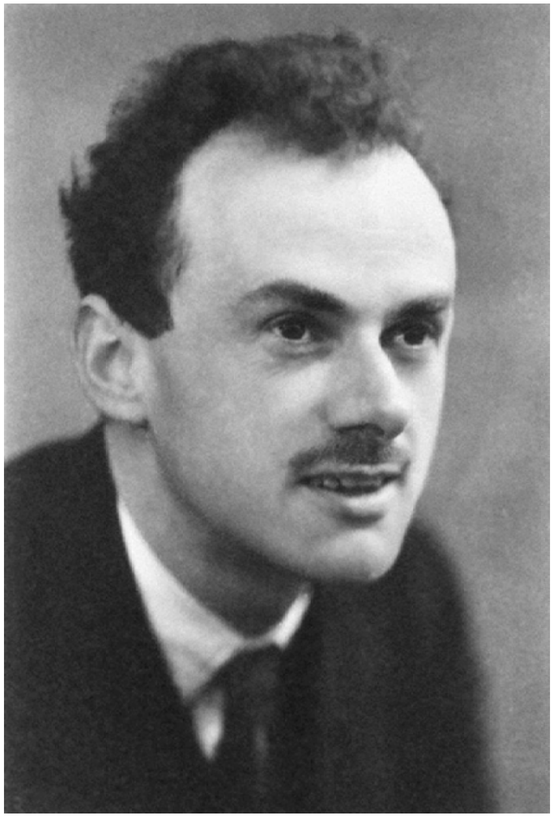


The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus **completely known**, and **the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.**

- *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, Vol. 123, No. 792* (6 April 1929)



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 $\left\{\begin{array}{l}\text{Spin}\\ \text{Spin component w/ respect to an axis}\end{array}\right\}$ quantized

→ Could be orbital spin

or intrinsic 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 $l = 1$ $\quad m_l = -1, 0, +1$

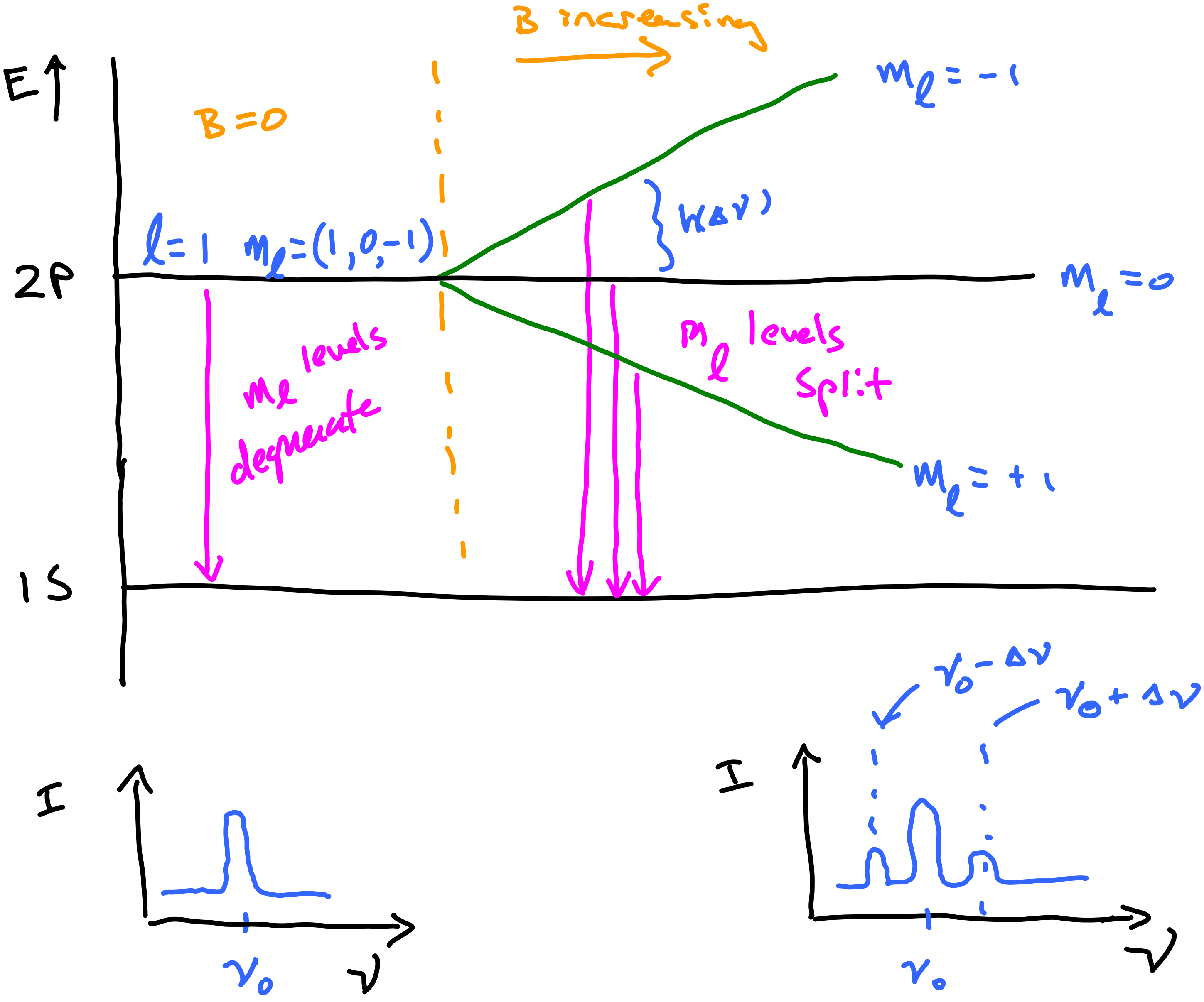
$$l_z = -1\hbar, 0, +\hbar$$

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

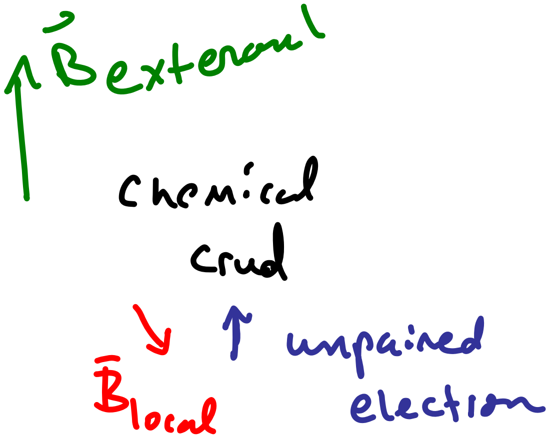
Bohr magneton $\equiv \mu_B$

Zeeman effect

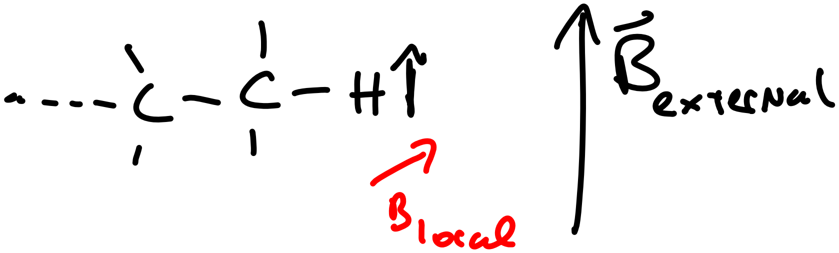
$U = -\mu_B m_\ell B$ For $\ell = 1$ $m_\ell = -1, 0, +1$



Electron Spin resonance



Nuclear Magnetic Resonance



Scan field . . . or scan frequency

Max Born German (1882-1970)

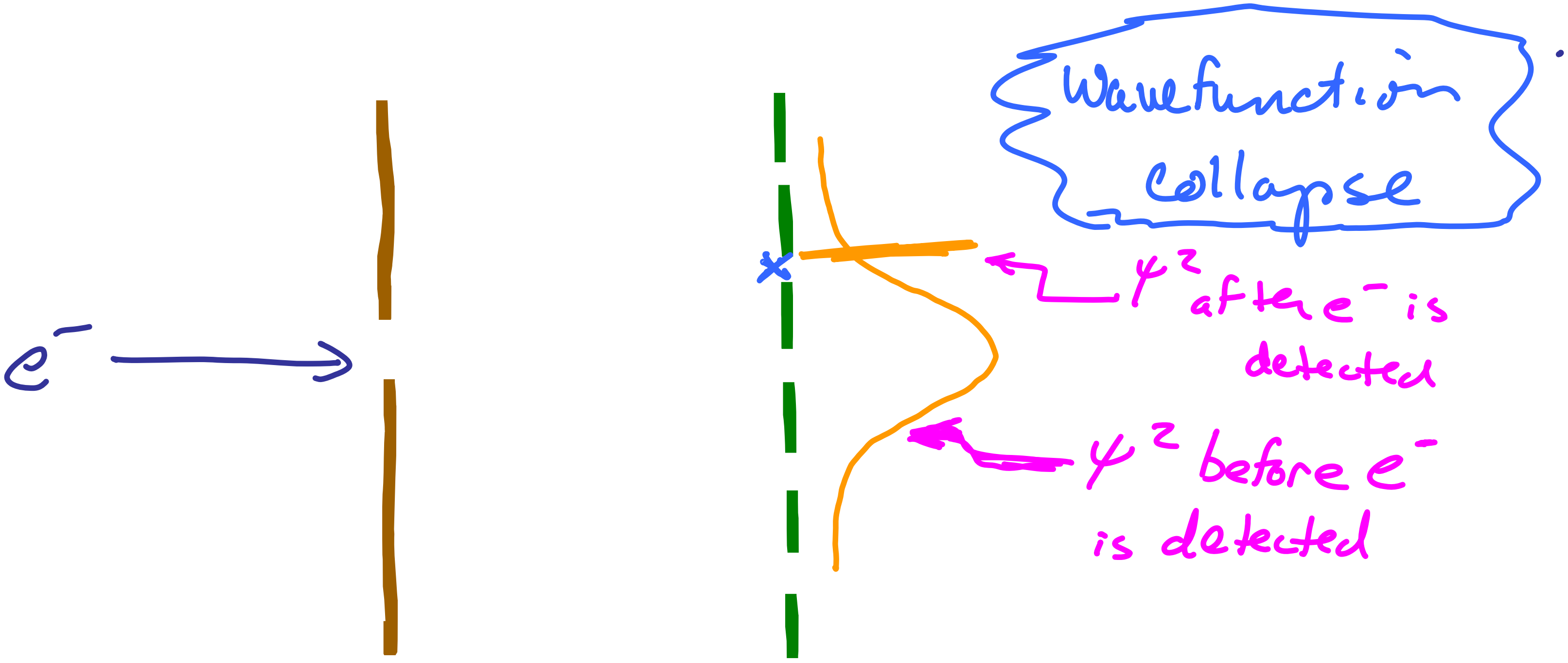
Note Title 2/26/2007

1954 Nobel Prize in physics

"For his fundamental research in quantum mechanics, especially for his statistical interpretation of the wavefunction"

$\psi(x)$ wave function

$\psi^2(x) \sim$ probability of finding particle in region of space



Once electron hits the film/Detector we know with 100% certainty where the electron hits
- So wavefunction has to "collapse"