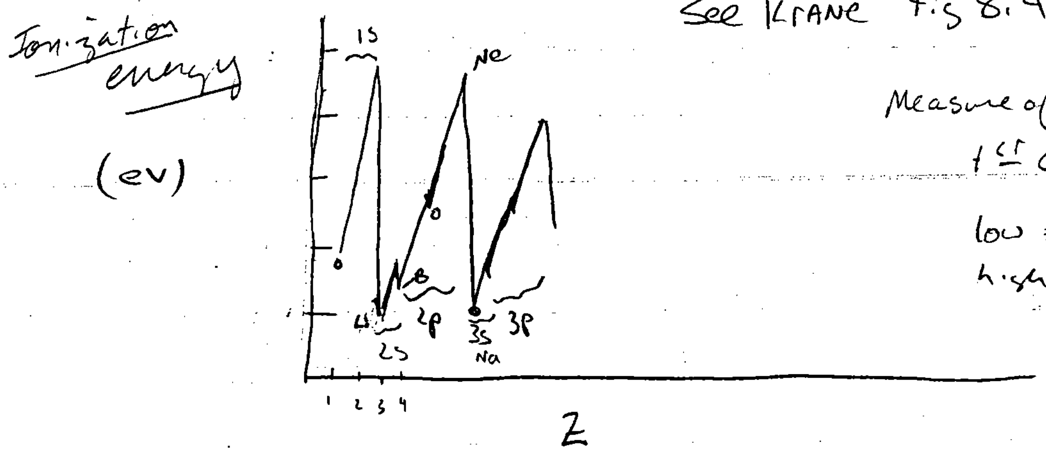
Periodic Chart reflects This structure:

Show chart from KRANE

Properties of chemical elements can be understood in terms of the Atomic level structure we are discussing

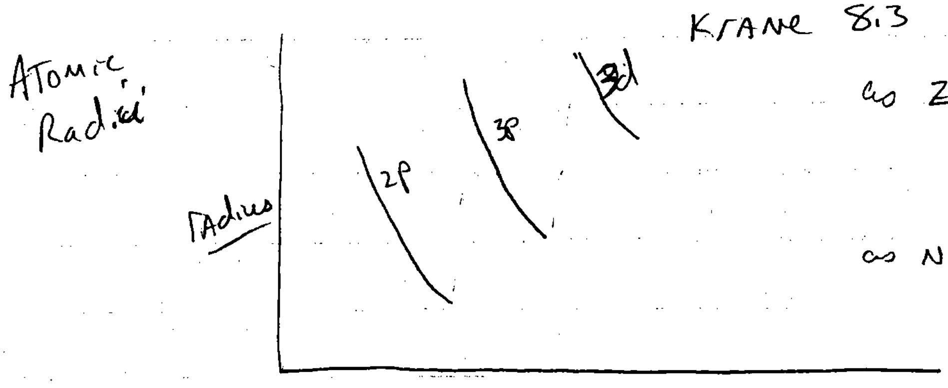
- Filled subshells, very stable configurations
  Normally do NOT contribute to "Chemistry"
- Atoms having 1 e^- over a filled shell will readily give that e^- up in a chemical reaction (lowers overall energy.
  Atoms lacking 1 e^- from a filled shell will react to gain that e^- to form a filled shell (more stable)



See KRANE Fig 8.4 p210

Measure of ease w/ which 1^{st} e^- given up

low ≡ easy
high ≡ hard



KRANE 8.3 p209

as Z increases within a shell
Atomic radius decreases

as New shell is added
Atomic radius increases

Bohr Atom $R \sim \frac{n^2}{Z}$

- H, Na are *very* reactive
- *Noble* gases He, Ne, Ar ... have filled levels
  are *very* inert chemically

Chemical bonds

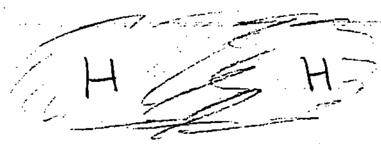
ionic bond – one ATOM takes e^- from another
$\Rightarrow$ both have filled shells (More Stable)
and are charged (attract each other

$Z=11$ Na [Ne] $3s^1$
$Z=17$ Cl [Ne] $3s^2 3p^5$

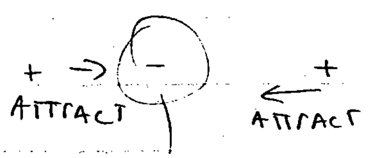
Na^+ [Ne] } *ions* ATTACT each other
$Cl^{\ominus}$ [Ar] } (electrostatic)
NaCl Table salT

Covalent bond

H_2



each H shares 2 electrons
$\Rightarrow$ Molecular orbital



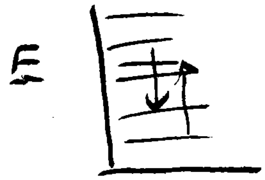
High $\ominus$ charge density in the middle

```
    H
    |
H – C – H
    |
    H
```

Methane (C needs 4 e^- to get to [Ne])
(H needs $2e^-$ to get to [He

~~Spectroscopy~~ Discrete energy levels

Key to understanding Atomic Structure



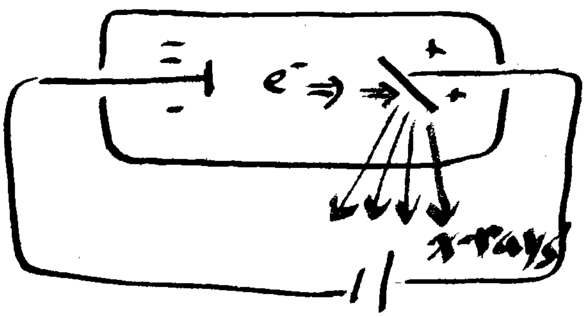
Transitions occur between allowed STATES

Permits a detailed Study of atomic Model, environment of Atom, Sample composition
(NMR) (Emission, Absorption spectra)
(ESR)

Many Applications: X rays, NMR, lasers ...

X-rays

1895 discovery Roentgen



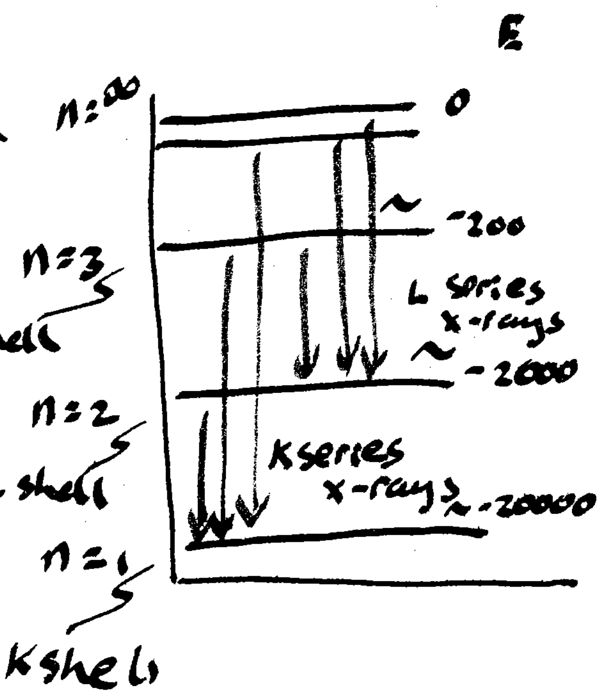
Cathode tube

Cathode rays

e^- incident on a high Z material

X-rays
$100 \sim 100{,}000$ eV $= h\nu$

overlaps w/ ultraviolet on the soft end
and gamma rays on the hard end



Principle — Chemistry, Biochemistry explained by quantum mechanics
— Forces at work basically understood

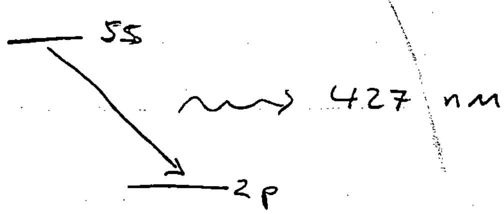
⇒ Chemists, Biologists not out of business
- Cannot solve QM of complex systems like medium sized molecules or dogs.
- New and unexpected phenomena come about with added complexity ⇒ Life

Key to understanding Atomic structure experimentally is spectroscopy

Many different kinds

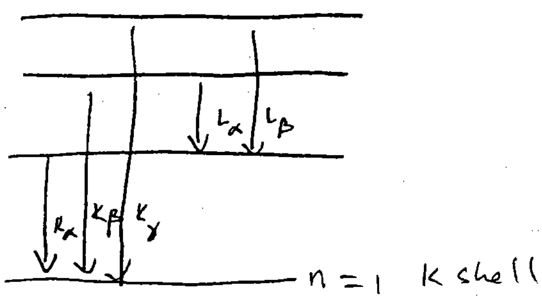
optical transitions occur in relatively loosely held outer shells

i.e.



(must obey selection rules) — conserve angular momentum and spin.

Xrays occur when tightly bound inner electron in high Z ~~election~~ Atom is ejected and one of the outer electrons makes a transition down to the lower shell

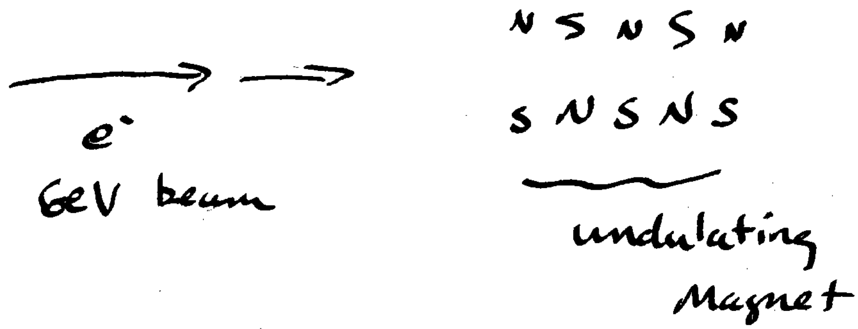


Calculate the energy Necessary to "ionize" heavy element with $Z = 40$ by removing e^- from $n=1$ shell

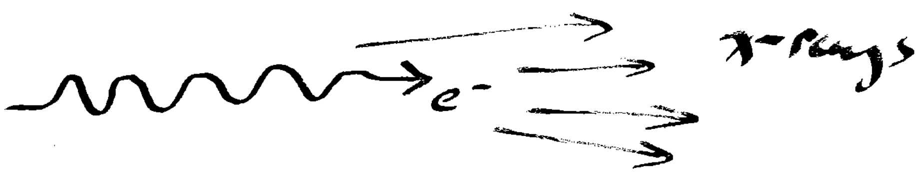
$$E_n \sim -\frac{Z^2}{n^2} E_0 \sim -40^2 (13.6\,eV) \cong 22000\ eV$$

$\Rightarrow$ this is the order of Magnitude for $E_{h\nu}$ emitted as electrons from outer shells cascade down to fill the hole

X rays also from high intensity light sources



from above



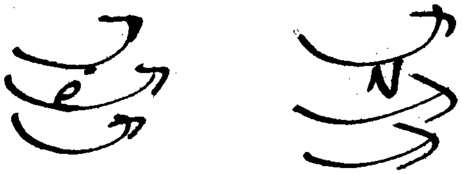
frequency determined by P_{e^-} and Spacing of Magnets

Very important source ~~for~~ of high intensity, high frequency ~~electron bea~~ x-ray beams for research

We will discuss absorption when we do Nuclear Physics.

Election Spin Resonance (ESR)
Nuclear Magnetic Resonance (NMR)

Recall



Particles can be thought of as "spinning" charge distributions w/ quantized "allowed" values of Angular Frequency

⇒ e^- point like as far as we know

⇒ Nuclei have structure

This is intrinsic spin ⇒ leads to a small magnetic moment
Acts like a small Dipole

~~[illegible]~~ I
intrinsic Angular Momentum I
Total spin $\frac{1}{2}$ for e^-
integer or ½ integer for Nuclei
$^{13}/_2$, 1 … etc.

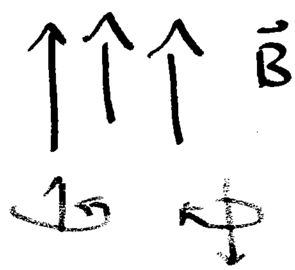
Spin Z component
$m = I, I-1, \dots -I$ $\quad e^- \quad \pm \frac{1}{2} = m_s$

Nuclei also ± Value

Determining Spin structure is important in Nuclear Structure expts

Spin can also be used as a diagnostic or tool for probing particle environment

Dipole in Magnetic field



Potential Energy in system Depends on the orientation of Dipole in B field

Let z direction be along $\vec{B}$

$$E_{Mag} = -g \mu B m$$

- m — z component of spin
- B — B magnitude
- g — constant (NOT gravity)
- μ — Magnetic moment of particle

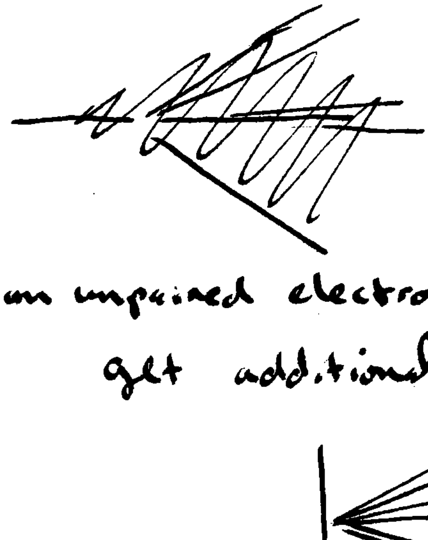
For $B = 0$

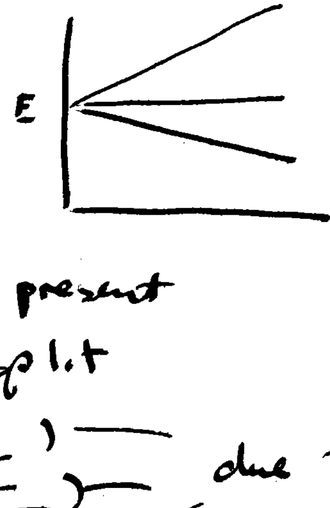
atoms/Nuclei w/ all M ~~at~~ in a given energy level are degenerate in energy

Atom $n = 3$ $l = 1$ $m_l = 1, 0, -1$ > all have same energy

$m_s = \pm 1/2$

Turn on B

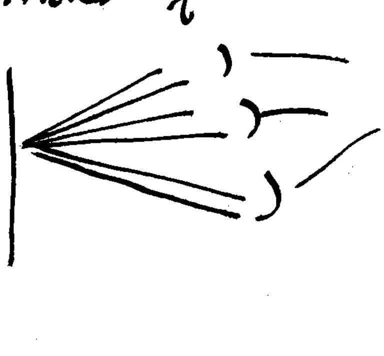




Split due to m_l

Zeeman Splitting

If an unpaired electron present get additional split

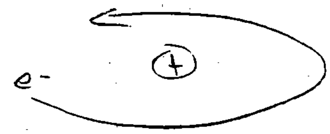


due to e^- spin B interaction

Spectroscopy in Magnetic fields / electric fields
important tools!

ex Zeeman Splitting

recall



little magnetic dipole created by e⁻ orbiting around nucleus

$$\vec{\mu}_\ell = \frac{\mu_b}{\hbar}\vec{L} = \left(\frac{e}{2M}\right)\vec{L}$$

Suppose we have an atom w/ e⁻ in 2p state (ignore e⁻ spin)

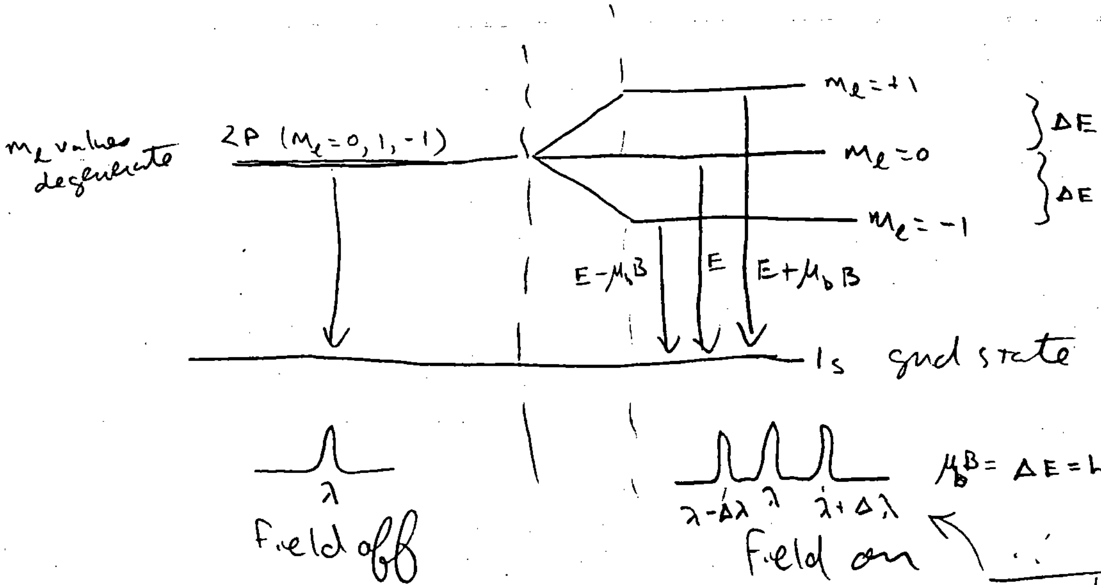
energy of interaction of μ with B = $V = -\vec{\mu}\cdot\vec{B}$

Let direction of B determine z axis

Then

$$V = \left(\frac{e}{2M}\right)\vec{L}\cdot\vec{B} = \frac{e}{2M}L_z B = \frac{e\hbar}{2M}m_\ell B = \mu_b m_\ell B$$

2P state $m_\ell = 1, 0, -1$

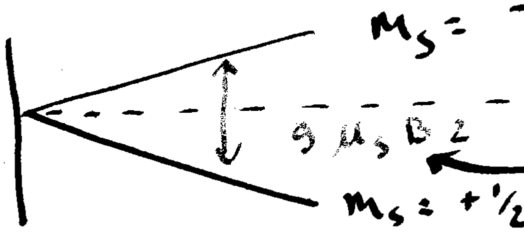


$$\mu_b B = \Delta E = h\Delta\nu = h\frac{c}{\Delta\lambda}$$

$\therefore$

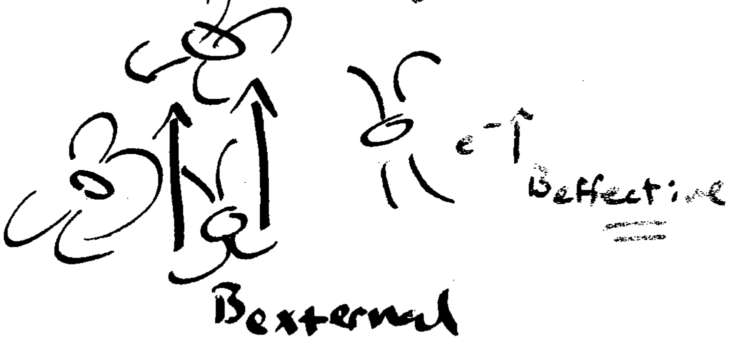
$$\boxed{\Delta\lambda = \frac{hc}{\mu_b B}}$$

Transitions between Zeeman levels would be at a diff frequency!

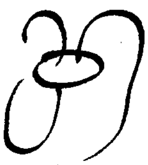


actual B at e^- NOT Necessarily applied B

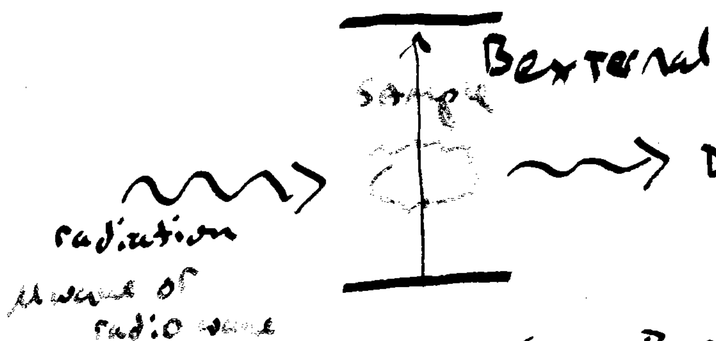
Usefulness in chemistry, biology



B effective Depends on the environment



Atoms w/ Dipole fields + Nuclei



Detector - Electron spin resonance ~~Dete~~ Signal

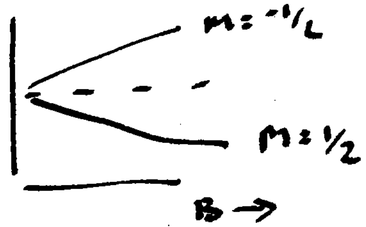
Scan B or $h\nu$ until have "resonance"

usually

Typical NMR

Put Sample in B field

E state of depends on orientation of Spin = 1/2 protons w/ respect to B



apply $h\nu$ to cause Transitions between two relative spin levels

exact $h\nu$ depends on B_{eff} ... dependson "Nuclear Environment"