Modern Physics

ATOMS AND MOLECULES

Topics We'll Cover

- Atomic Structure
- The Bohr Atom
- Energy Levels
- Atomic Spectra
- Franck-Hertz Experiment
- Laser
- Rutherford Scattering

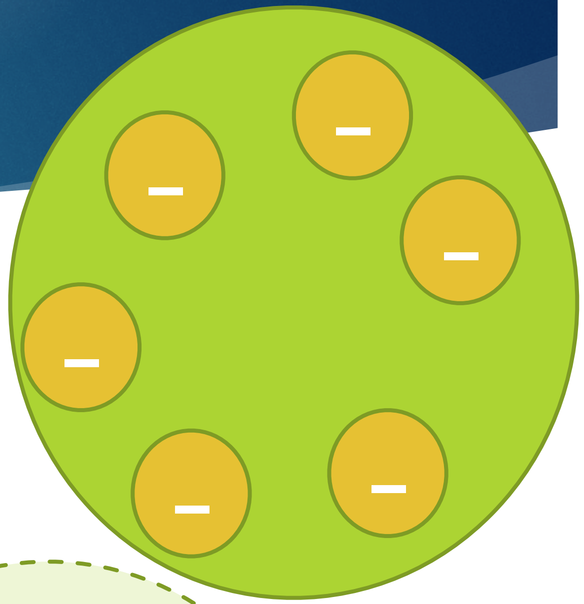
Visiting Labs

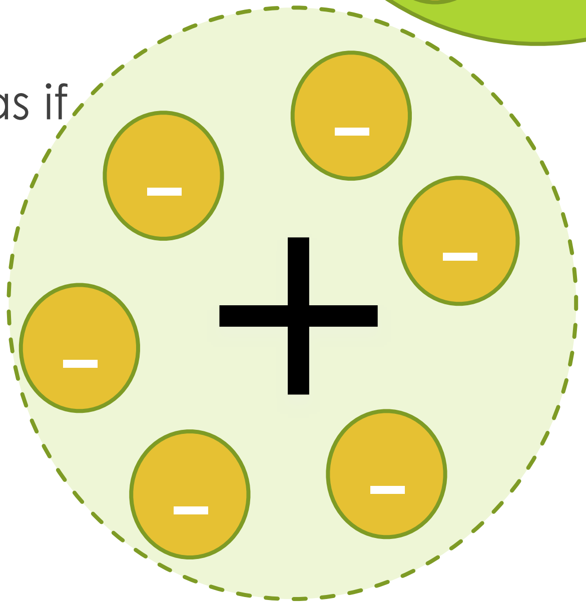
- At NTUT
- At Academia Sinica

Atomic Structure

- Plum pudding (fruitcake) model or Thomson's model of the atom – investigated from alpha particle scattering at gold foil, with signals on a zinc sulfide screen (which emits light when struck by the .)
  - Thomson writes in the Philosophical Magazine 1904, "... the atoms of the elements consist of a number of negatively electrified corpuscles enclosed in a sphere of uniform positive electrification, ..."
- Rutherford, Thomson's student, noticed that "It was incredible as if you fired a 15-inch shell at a piece of tissue paper and it came back and hit you." So he updated the model to
  - Rutherford's model: tiny positively charged nucleus

  with electron cloud nearby





Atomic Structure

- The detector measures alpha particles scattered between θ and $\theta + d\theta$. Let's figure out the scattering angle.
- From impulse and momentum conservation, $\Delta p = p_2 - p_1 = \int F\, dt$. So p_1=p_2=mv. From the law of sines, the geometry tells us that $\frac{\Delta p}{sin\theta} = \frac{mv}{sin\frac{\pi-\theta}{2}}$ $and\ since \sin\frac{1}{2}(\pi-\theta) = \cos\frac{\theta}{2}$, $sin\theta = 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}$. $Thus,\ \ \Delta p = 2mv\ sin\frac{\theta}{2}$.
- Because the impulse is in the direction of momentum change, $\left|\int Fdt\right| = \int Fcos\phi dt$.
- Equating the terms, $2mvsin\frac{\theta}{2} = \int_{-\frac{\pi-\theta}{2}}^{+\frac{\pi-\theta}{2}} Fcos\phi \frac{dt}{d\phi} d\phi$.
- The electric force exerted by the nucleus on the alpha particle acts along the radius vector joining them, so there is no torque on the alpha particle and its angular momentum is constant.
- $-m\omega r^2 = mr^2 d\phi\backslash dt = mvb$. $So\ 2mv^2 b\sin\frac{\theta}{2} = \int_{-\frac{\pi-\theta}{2}}^{+\frac{\pi-\theta}{2}} Fr^2 cos\phi d\phi$. From $F = \frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{r^2}$ we then derive
- $cot\frac{\theta}{2} = \frac{2\pi\epsilon_0 mv^2}{Ze^2} b = \frac{4\pi\epsilon_0 KE\ b}{Ze^2}$

Fig. 4.3 Textbook

Atomic Structure

- Cross section for scattering is $\sigma = \pi b^2$
- The foil contains n number of atoms per unit volume with thickness t. So in an area A, ntA nuclei are present for scattering. $ntA\sigma$ is the total cross section. The question to ask is what fraction of nuclei scatters an alpha particle,
$$f = \frac{alpha\ particles\ scattered\ by\ \theta\ or\ more}{incident\ alpha\ particles} = \frac{total\ cross\ section}{target\ area} = \frac{ntA\sigma}{A} = nt\pi \mathrm{b}^2$$
- $$f = \pi nt\left(\frac{Ze^2}{4\pi\epsilon_0 KE}\right)^2 cot^2\frac{\theta}{2}$$
- The fraction depends on the scattering angle, atomic and nuclei number, the kinetic energy, and the thickness of the foil.

Atomic Structure

- The detector measures alpha particles scattered between θ and $\theta + d\theta$. The fraction of incident alpha particles scattered in this finite range is
- $$df = -\pi n t \left(\frac{Ze^2}{4\pi\epsilon_0 KE} \right)^2 cot\frac{\theta}{2}\csc^2\frac{\theta}{2} d\theta$$
- The area the particles strike is

$$dS = (2\pi r \sin\theta)(r\ d\theta) = 2\pi r^2 sin\theta d\theta = 4\pi r^2 \sin\frac{\theta}{2}\cos\frac{\theta}{2}\ d\theta$$

- The number N per unit area striking the screen at angle, which is the actual measured physical quantity, is:
- $$N(\theta) = \frac{N_i \left| df \right|}{dS} = \frac{N_i \pi n t \left(\frac{Ze^2}{4\pi\epsilon_0 KE} \right) \cot\frac{\theta}{2}\csc^2\frac{\theta}{2}\ d\theta}{4\pi r^2 \sin\frac{\theta}{2} cos\frac{\theta}{2} d\theta} = \frac{N_i n t Z^2 e^4}{\left(8\pi\epsilon_0\right)^2 r^2 KE^2 \sin^4\frac{\theta}{2}}$$
- Notably, only 0.14 percent of the incident alpha particles are scattered by more than 1 degree. This formula described well the observations of Geiger and Madsen, Rutherford's students.

Fig. 4.33 textbook

Atomic Structure – An Example

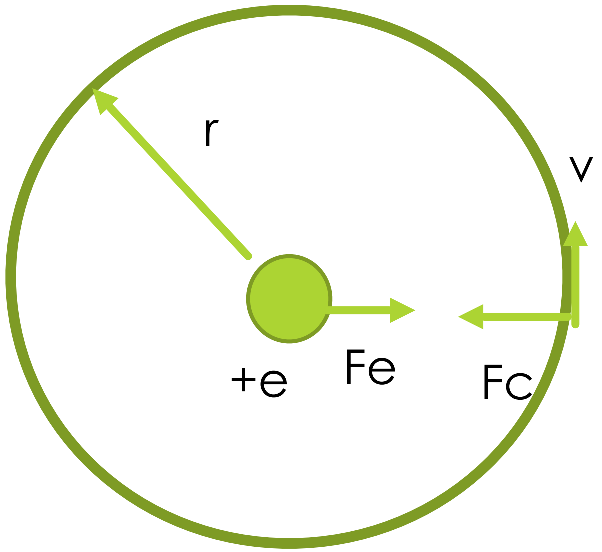
- From the assumption that the kinetic energy equals the potential energy, the distance of closest approach is estimated. This is the distance of closest approach for the most energetic alpha particle that hits the gold foil.
- $$R = \frac{2Ze^2}{4\pi\epsilon_0 KE} = \frac{2 * 9.0 * \frac{10^9 Nm^2}{C^2} * \left(1.6 * 10^{-19} C\right)^2 * Z}{1.2 * 10^{-12} J} = 3.8 * 10^{-16} Zm = 3.8 * 10^{-16} * 79\ m = 3 * 10^{-14} m\,.$$
- At higher and higher energies > 7.7 MeV, Rutherford’s description becomes less precise, and in fact the gold radius is found to be 1/5 this value.
- Why is this? Let’s consider electron screening and orbits.

Electron Orbits – An example

- Experiments indicate that 13.6 eV is required to separate a hydrogen atom into a proton and an electron; that is, its total energy is E = -13.6 eV. What is the orbital radius and velocity of the electron in a hydrogen atom?
- Since 13.6 eV = 13.6 * 1.6 * 10^{-19} J = 2.2 * 10^{-18} J. Then

$$r = -\frac{e^2}{8\pi\epsilon_0 E} = 5.3 \ast 10^{-11}\ m\,.$$

- The velocity is estimated $v = \frac{e}{\sqrt{4\pi\epsilon_0 m r}} = 2.2 \ast 10^{6}\ m/s.$



The Bohr Atom

My Problem 4 – A RAP

Einstein n Bohr, talkin together
Fysicists they flockin birds of a feather
Wondering bout the universe keys
At the speed of light, wut do you C?
Correspondence to that is the light quantum
Scale so small that's hard to fathom
But just as we slow an so things get big.
We recover the classics, maybe just trig'
You n me all thaz bout, aight peace out.
Dig?

The Bohr Atom

- Concept put forward by Niels Bohr in 1913, assuming one proton and one electron.
- Starting with the de Broglie wavelength, we write: $\lambda = \frac{h}{mv} \rightarrow v = \frac{c}{\sqrt{4\pi\epsilon_0 mr}} \rightarrow \lambda = \frac{h}{e}\sqrt{\frac{4\pi\epsilon_0 r}{m}}$. We can use this formula to estimate the electron wavelength to be 33 * 10^{-11} m, assuming an electron orbit of r = 5.3 * 10^{-11} m. Note that $2\pi r$ = 33 * 10^{-11} m! This means that the electron orbit in a hydrogen atom is one electron wavelength in circumference.
- *An electron can circle a nucleus only if its orbit contains an integral number of de Broglie wavelengths.* $n\lambda = 2\pi r_n, \quad n = 1,2,3,\ldots$
- The quantum number n is part of the equation for the orbit stability and orbital radii: $\frac{nh}{e}\sqrt{\frac{4\pi\epsilon_0 r_n}{m}} = 2\pi r_n \rightarrow r_n = \frac{n^2 h^2 \epsilon_0}{\pi m e^2} = \ with\ r_1 = a_0 = 5.292\ * 10^{-11}\ m,\ the\ Bohr\ radius,\ while\ r_n = n^2 a_0$.

Energy Levels in an Atom

- This basic model describes the single proton, single electron Hydrogen atom. Using the concept of quantized number of levels in the circular orbit, the energy (of electrons) permitted in the various orbits can be estimated.
- This achievement helps to build the periodic table known to us.
- $$E_n = \frac{e^2}{8\pi\epsilon_0 r_n} = -\frac{me^4}{8\epsilon_0^2 h^2}\frac{1}{n^2} = \frac{E_1}{n^2} = -13.6\frac{eV}{n^2}$$
- Spectral lines from (hydrogen) atom emission give rise to the following observations

Excited states

Fig. 4.15 textbook

Ground state

Energy Levels in an Atom – Origin of Line Spectra

- Spectral lines from (hydrogen) atom emission give rise to the following observations, which are described with these sequences.
- $Lyman\colon n_f = 1\colon \frac{1}{\lambda} = -\frac{E_1}{ch}\left(\frac{1}{1} - \frac{1}{n^2}\right)$
- $Balmer\colon n_f = 2\colon \frac{1}{\lambda} = -\frac{E_1}{ch}\left(\frac{1}{4} - \frac{1}{n^2}\right)$
- $Paschen\colon n_f = 3\colon \frac{1}{\lambda} = -\frac{E_1}{ch}\left(\frac{1}{9} - \frac{1}{n^2}\right)$
- $Brackett\colon n_f = 4\colon \frac{1}{\lambda} = -\frac{E_1}{ch}\left(\frac{1}{16} - \frac{1}{n^2}\right)$
- $Pfund\colon n_f = 5\colon \frac{1}{\lambda} = -\frac{E_1}{ch}\left(\frac{1}{25} - \frac{1}{n^2}\right)$

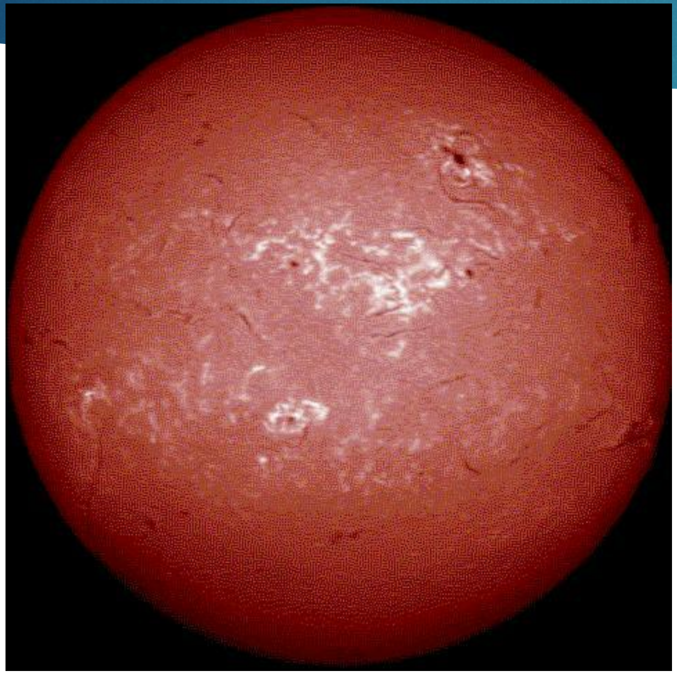
e- says, "I'm free"

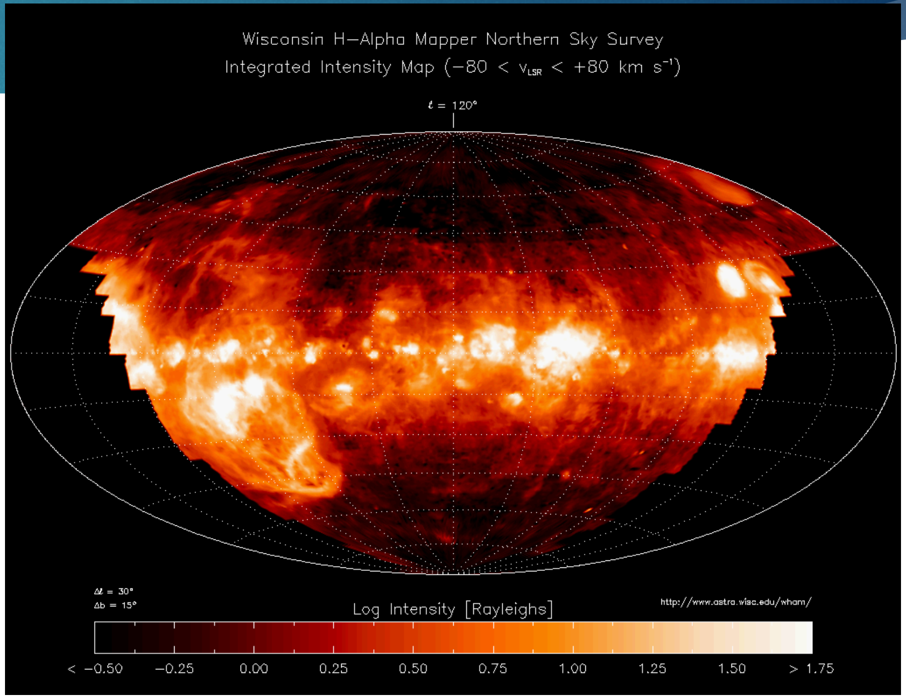
Fig. 4.16 textbook

Emissions

- Find the longest wavelength present in the Balmer series of hydrogen, corresponding to the Hα line.
- $\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) = R\left(\frac{1}{2^2} - \frac{1}{3^2}\right) = 0.139R \rightarrow \lambda = 656\ nm$

Emissions





- An **H-alpha filter** is an optical filter designed to transmit a narrow bandwidth of light generally centred on the H-alpha wavelength.[2] These filters can be dichroic filters manufactured by multiple (~50) vacuum-deposited layers. These layers are selected to produce interference effects that filter out any wavelengths except at the requisite band.[3] The Sun observed through an optical telescope with an H-alpha filter.

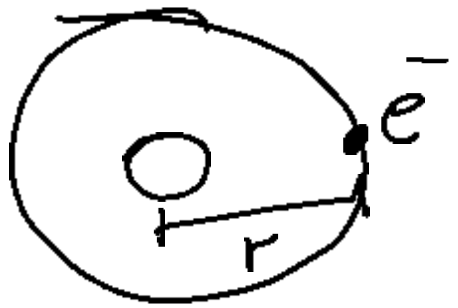
A Milky Way view by Wisconsin H-Alpha Mapper survey

Nuclear Motion and Nuclear Mass

- We should now realize that motion and mass both have effects on the wavelengths (of spectral lines) observed.
- For example, let's consider a positronium "atom" that is a system of positron and electron that orbit each other. Let's compare the wavelengths of the spectral lines of positronium with ordinary hydrogen.
- $m' = \frac{mM}{m+M} = \frac{m^2}{2m} = \frac{m}{2}$, *with m the electron mass . Then* $E_n' = \frac{\left(\frac{m'}{m}\right)E_1}{n^2} = \frac{E_1}{2n^2}$.
- This means the Rydberg constant, for positronium is half as large as it is for ordinary hydrogen, and thus, the wavelengths of positronium spectral lines are all twice those of the corresponding lines in the hydrogen spectrum.

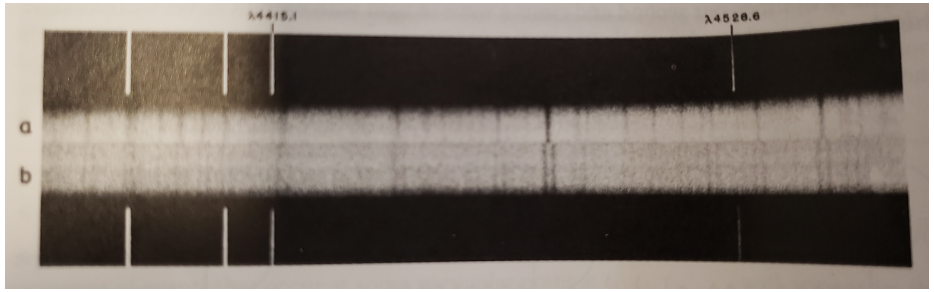
Nuclear Motion and Nuclear Mass

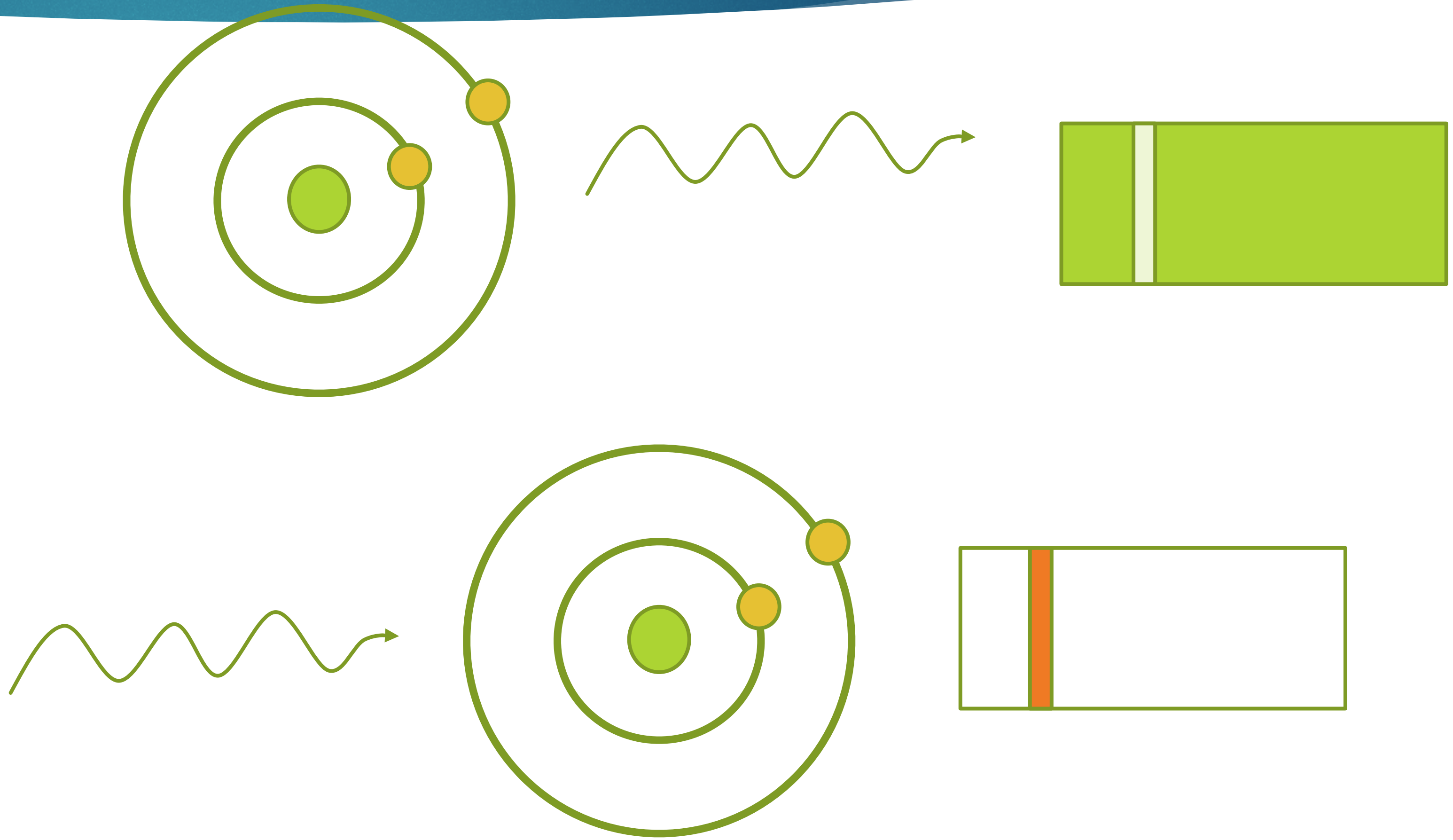
- A muon is an unstable elementary particle whose mass is 207 m_e, with charge +e or –e. A negatively charged muon can combine with a proton to create a muonic atom.
- The reduced mass is $m' = \dfrac{mM}{m+M} = \dfrac{207m_e 1836m_e}{207m_e + 1836m_e} = 186m_e$
- The radius of orbit is $r_1 = \dfrac{h^2\epsilon_0}{\pi m_e e^2}$
- For n=1 and r_1=a_0=5.29*10^{-11} m, we have $r_1' = \dfrac{m}{m'}r_1 = \dfrac{m_e}{186m_e}a_0 = 2.85 * 10^{-13}m$.
- The muon is 186 times closer to the proton than an electron would be.
- Ionization energy $E_1' = \dfrac{m'}{m}E_1 = 186E_1 = -2.53 * 10^3 eV$



Atomic Excitation

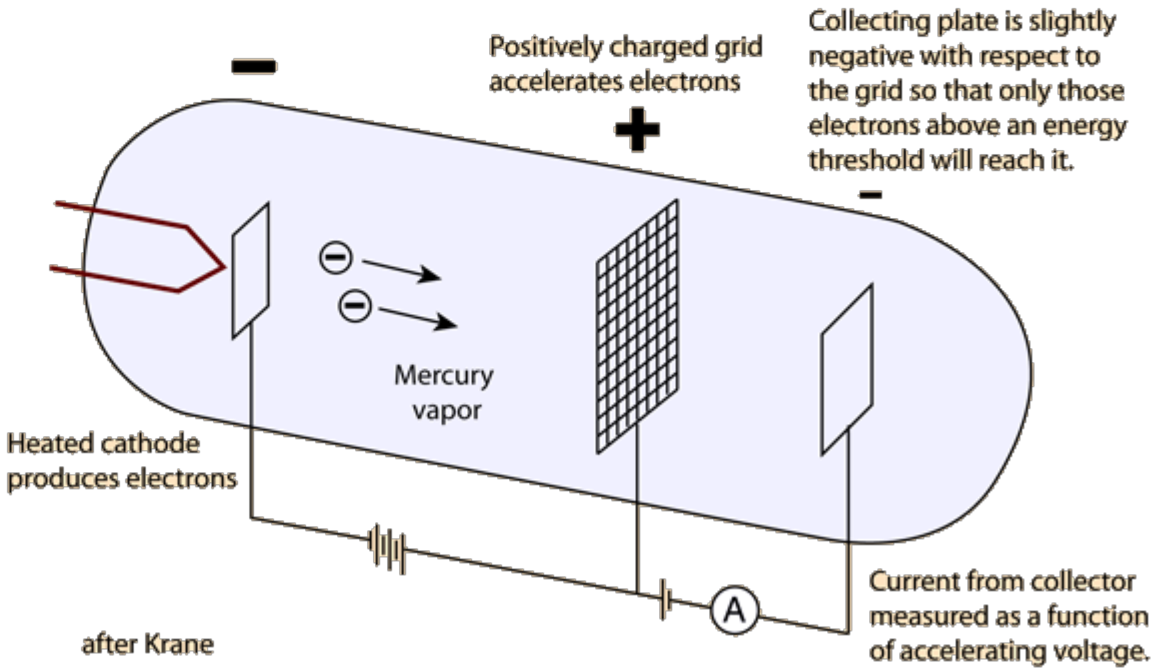
- The origin of atomic emission/absorption spectral lines

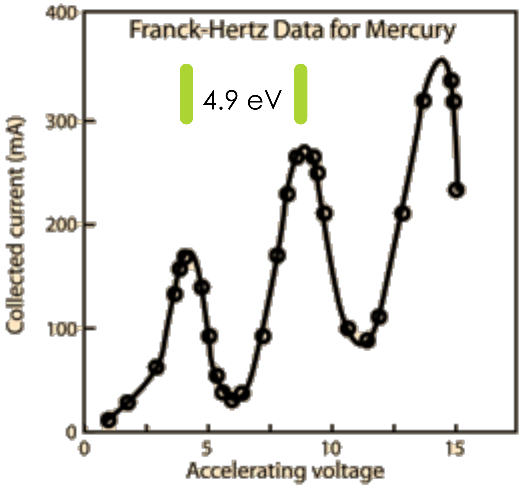


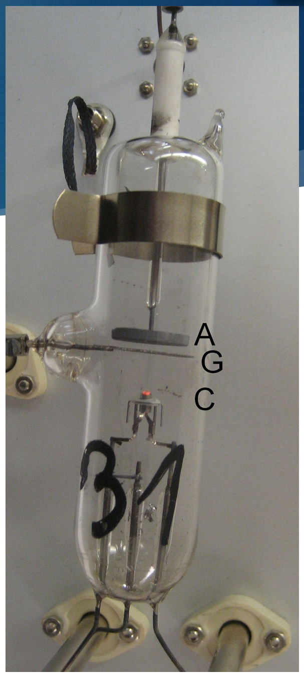


Franck-Hertz Experiment

- Confirmation of Bohr's basic ideas, that a minimum electron energy needed to excite spectral lineshapes.
- For mercury, 254 nm emission from the 4.9 eV excitation.

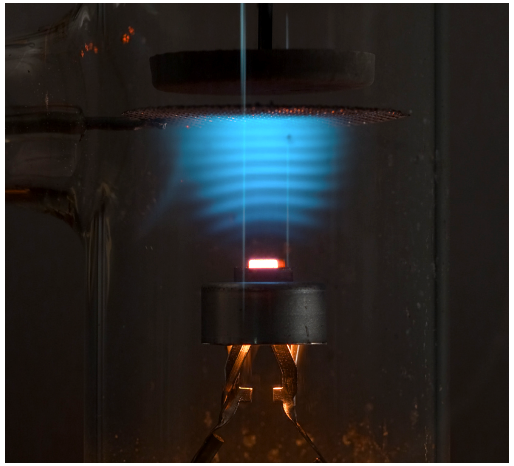






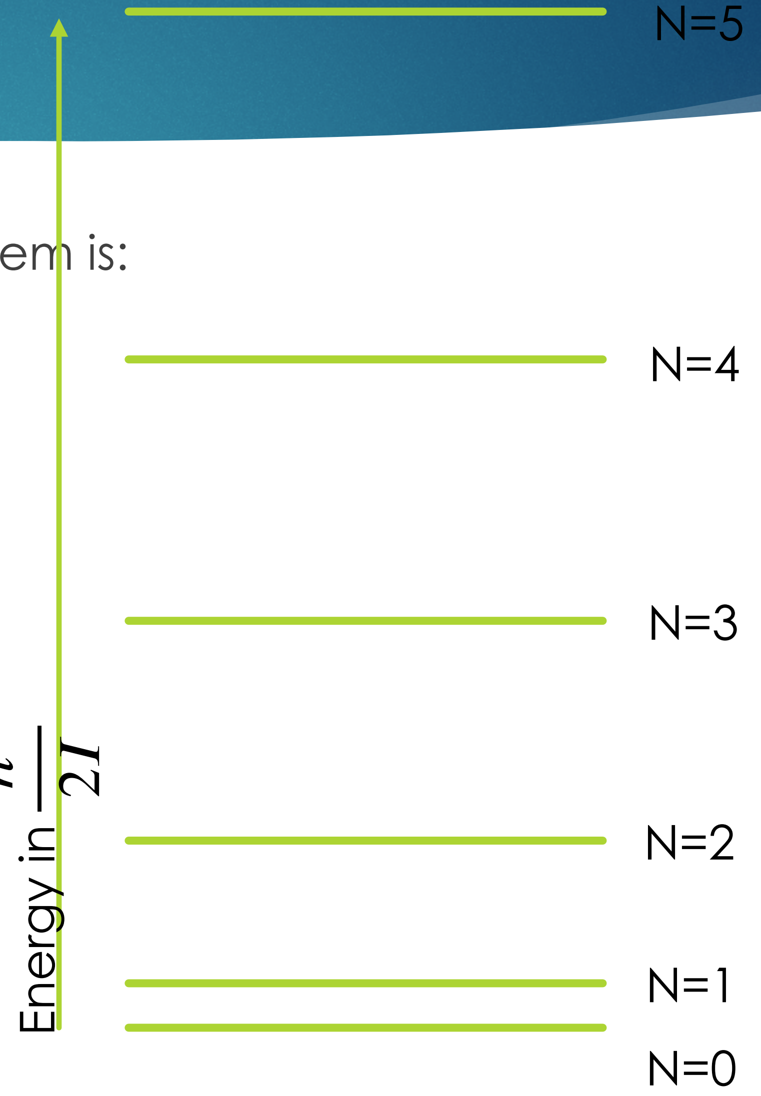
Apparatus for Mercury
C cathode
G mesh
A anode

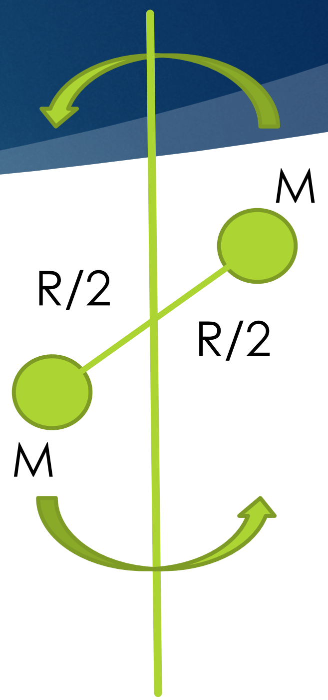
Hg vapor triode



Rotations to Diatomic Molecules

- The rotational inertia of this dumbbell system is:
- $I = M\left(\frac{R}{2}\right)^2 + M\left(\frac{R}{2}\right)^2 = \frac{MR^2}{2}$
- The angular momentum is found with
- $L = I\omega = \left(\frac{MR^2}{2}\right)\omega;\ E = \frac{L^2}{2I}$
- If the energy values are quantized, then
- $L = n\hbar$



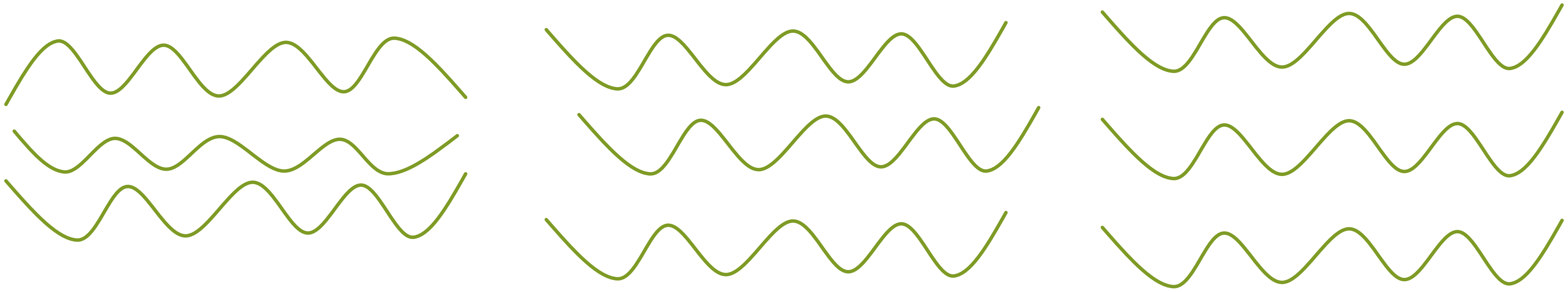


Rotations to Diatomic Molecules

- An example is Cl_2 , which has an average separation of 1.99 * 10^{-10} m between chlorine atoms. The atoms have nuclei which consist of 17 protons and 20 neutrons; suppose the same mass 1.67 * 10^{-27} kg. What is the separation in eV between the energies of the rotational ground state and the first excited state of this molecule?
- $$E_1 - E_0 = E_1 = \frac{\hbar^2}{mR^2} = \frac{(1.05 * 10^{-34}\ Js)\text{^}2}{37 * 1.67 * 10^{-27} kg\ * \left(1.99 * 10^{-10} m\right)^2} = \frac{4.19 *\ 10^{-24} J}{1.6 * 10^{-19} J} = 2.62 * 10^{-5} eV$$
- This spacing is more than 10000 times smaller than the typial 1 eV spacing of electronic levels in hydrogen.

Light Amplification From Stimulated Emission of Radiation

- The laser!

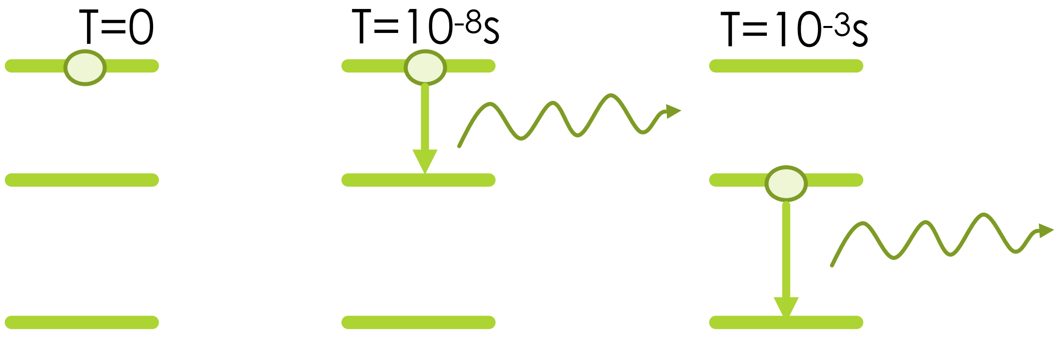


Ordinary light | Monochromatic, incoherent | Monochromatic Coherent light

Ordinary Excited State

Metastable state

Ground state

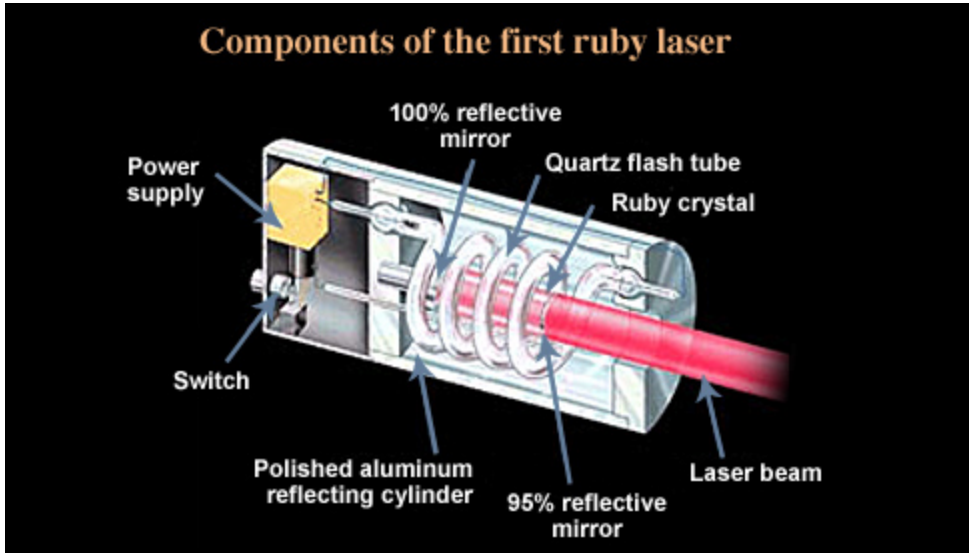


Induced absorption – aborbing photon and raising eneryg

Spontaneous emission – lowering of energy with light emission

Induced emission – enhanced beam of coherent light

Ruby Laser



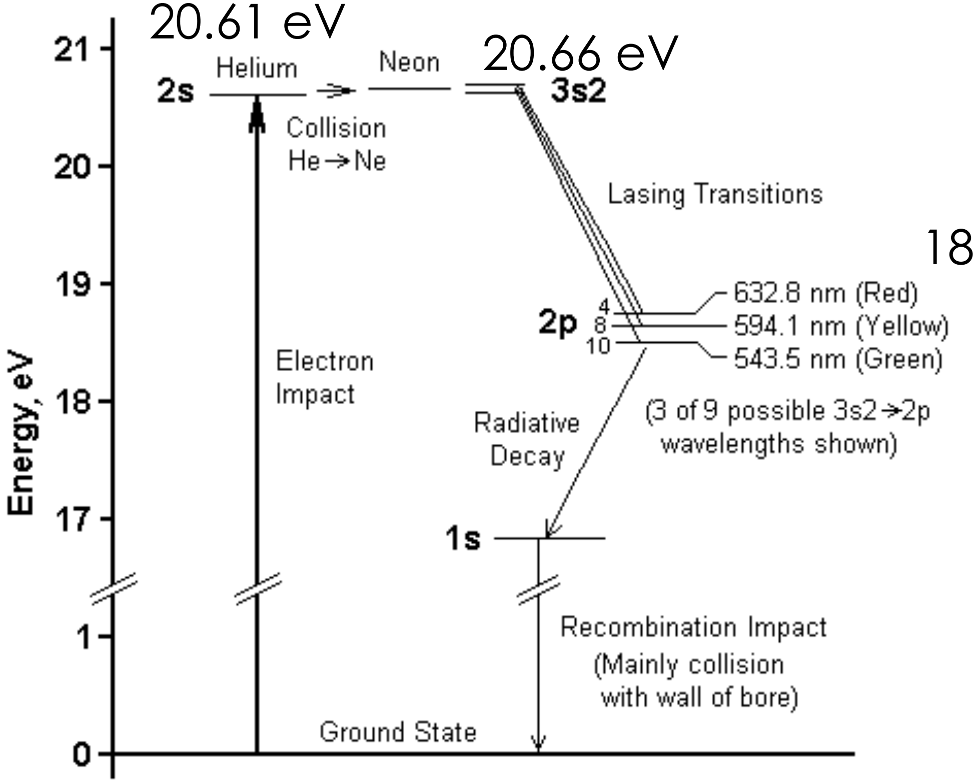
https://eurekaphysics.wordpress.com/experimental-physics/laser/ruby-laser/

Helium Neon Laser

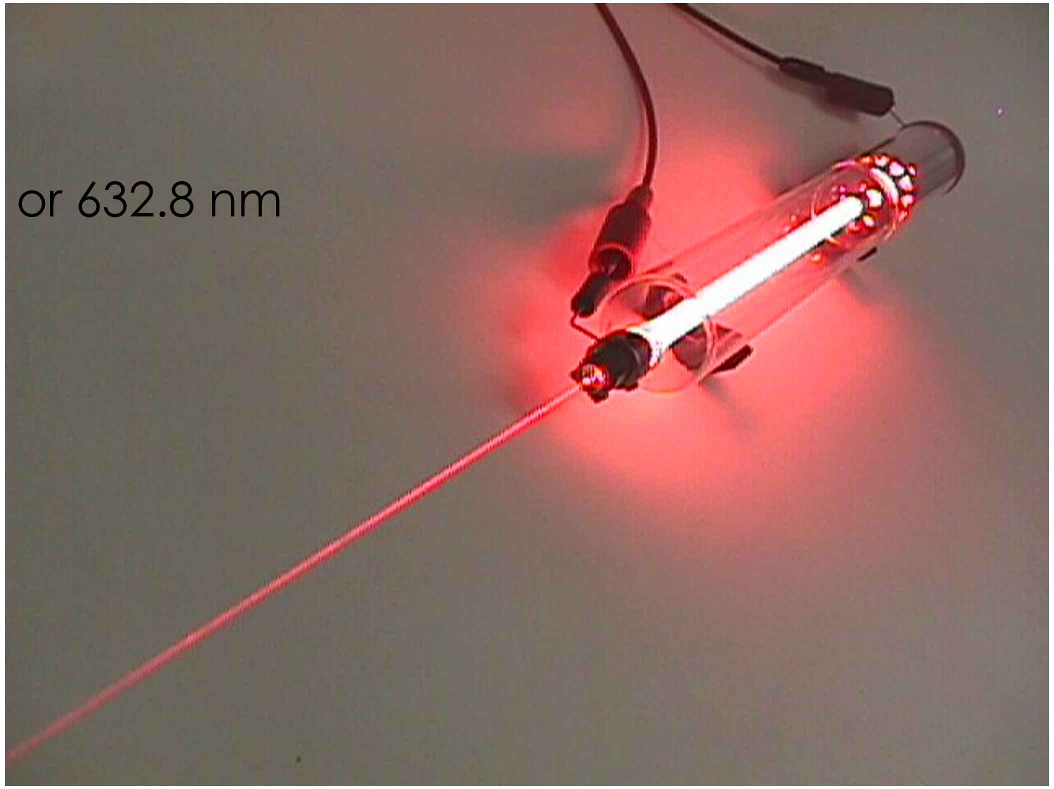
20.61 eV

20.66 eV

18.70 eV or 632.8 nm

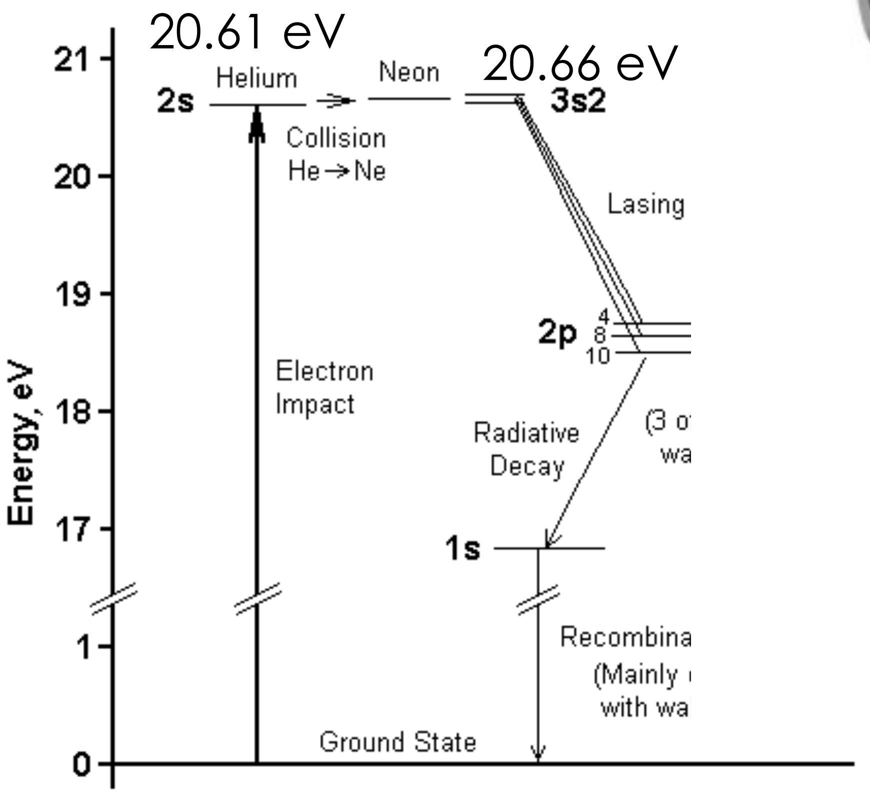


Helium-Neon Excitation and Lasing Process



https://eurekaphysics.wordpress.com/experimental-physics/laser/helium-neon-laser/

Helium Neo



Helium-Neon Excitation and Lasing Process

https://eurekaphysics.wordpress.com/experimental-physics/laser/helium-neon-laser/

Other Lasers

- Chemical lasers
- Dye lasers
- Carbon dioxide gas laser - 100 W output are helpful in surgery because they seal small blood vessels while cutting through tissue by vaporizing water in the path of their infrared beams.
- Semiconductor lasers

Electron Probability Distribution

$|\psi|^2$

Fig. 6.12 textbook

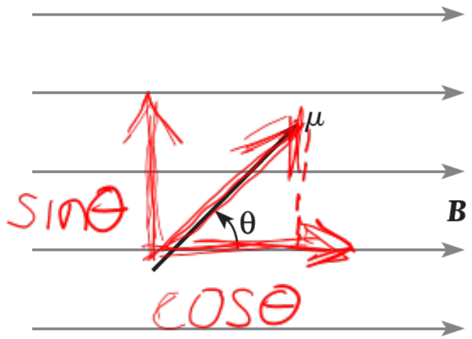
Zeeman Effect

- In a magnetic field, the electron, proton and neutron (?) interact with a magnetic field.
- Hence an energy arising from torque tau is generated on the particle.
- The particles such as the electron has an intrinsic magnetic moment.
- For an atom, the magnetic energy experienced is

$$U_m = \int_{\pi/2}^{\theta} \tau \, d\theta = \mu B \int_{\pi/2}^{\theta} \sin\theta \, d\theta$$

$$= -\mu B \cos\theta$$

$$\mu = -\left(\frac{e}{2m}\right)\mathbf{L}$$



$$U_m = m_l \left(\frac{e\boxed{?}}{2m}\right) B \qquad \mu_B = \frac{e\boxed{?}}{2m} = 9.274 \times 10^{-24} \text{ J/T} = 5.788 \times 10^{-5} \text{ eV/T}$$

Zeeman Effect

- Transition between levels in an atom under external magnetic field are then described by these frequencies.
- Features as these can be measured, for example, a 0.3 T magnetic field will generate a 0.00283 nm spacing in the spectral lines at 450 nm.

$$\nu_1 = \nu_0 - \mu_B \frac{B}{h} = \nu_0 - \frac{e}{4\pi m} \boxed{B}$$

$$\nu_2 = \nu_0$$

$$\nu_3 = \nu_0 + \mu_B \frac{B}{h} = \nu_0 + \frac{e}{4\pi m} B$$

Fig. 6.17 textbook

Rydberg Binding Energies

Fig. 7.8 textbook

Spin

- The Stern-Gerlach Experiment.

Hund's Rule

- A principle that in general the electrons in a subshell remain unpaired (so as to maintain a lowest energy state).
- This is related to the Pauli exclusion principle of atomic electrons (like charges repel). Electrons with same spin in same subshell have different m_l values and thus have wavefunctions whose spatial distributions are different.

The Periodic Table of the Elements

Table 7.2

The Periodic Table of the Elements

The number above the symbol of each element is its atomic number, and the number below its name is its average atomic mass. The elements whose atomic masses are given in parentheses do not occur in nature but have been created in nuclear reactions. The atomic mass in such a case is the mass number of the most long-lived radioisotope of the element.

Elements with atomic numbers 110, 111, 112, 114, and 116 have also been created but not yet named.

Transition metals

Group	1	2											3	4	5	6	7	8
Period 1	1 H Hydrogen 1.008																	2 He Helium 4.003
2	3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.81	6 C Carbon 12.01	7 N Nitrogen 14.01	8 O Oxygen 16.00	9 F Fluorine 19.00	10 Ne Neon 20.18
3	11 Na Sodium 22.99	12 Mg Magnesium 24.31											13 Al Aluminium 26.98	14 Si Silicon 28.09	15 P Phosphorus 30.97	16 S Sulfur 32.07	17 Cl Chlorine 35.45	18 Ar Argon 39.95
4	19 K Potassium 39.10	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titanium 47.88	23 V Vanadium 50.94	24 Cr Chromium 52.00	25 Mn Manganese 54.94	26 Fe Iron 55.8	27 Co Cobalt 58.93	28 Ni Nickel 58.69	29 Cu Copper 63.55	30 Zn Zinc 65.39	31 Ga Gallium 69.72	32 Ge Germanium 72.59	33 As Arsenic 74.92	34 Se Selenium 78.96	35 Br Bromine 79.90	36 Kr Krypton 83.80
5	37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.1	45 Rh Rhodium 102.9	46 Pd Palladium 106.4	47 Ag Silver 107.9	48 Cd Cadmium 112.4	49 In Indium 114.8	50 Sn Tin 118.7	51 Sb Antimony 121.9	52 Te Tellurium 127.6	53 I Iodine 126.9	54 Xe Xenon 131.8
6	55 Cs Cesium 132.9	56 Ba Barium 137.3		72 Hf Hafnium 178.5	73 Ta Tantalum 180.9	74 W Tungsten 183.9	75 Re Rhenium 186.2	76 Os Osmium 190.2	77 Ir Iridium 192.2	78 Pt Platinum 195.1	79 Au Gold 197.0	80 Hg Mercury 200.6	81 Tl Thallium 204.4	82 Pb Lead 207.2	83 Bi Bismuth 209.0	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
7	87 Fr Francium (223)	88 Ra Radium 226.0		104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Ns Nielsbohrium (262)	108 Hs Hassium (264)	109 Mt Meitnerium (266)									

Halogens Inert gases

Alkali metals

Lanthanides (rare earths)

57 La Lanthanum 138.9	58 Ce Cerium 140.1	59 Pr Praseodymium 140.9	60 Nd Neodymium 144.2	61 Pm Promethium (145)	62 Sm Sarnarium 150.4	63 Eu Europium 152.0	64 Gd Gadolinium 157.3	65 Tb Terbium 158.9	66 Dy Dysprosium 162.5	67 Ho Holmium 184.9	68 Er Erbium 167.3	69 Tm Thulium 168.9	70 Yb Ytterbium 173.0	71 Lu Lutetium 175.0
89 Ac Actinium (227)	90 Th Thorium 232.0	91 Pa Protactinium 231.0	92 U Uranium 238.0	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (260)	102 No Nobelium (259)	103 Lw Lawrencium (262)

Actinides

Examples

- J = L + S with $L = \hbar\sqrt{(L(L+1))}; S = \hbar\sqrt{(S(S+1))}; J = \hbar\sqrt{(J(J+1))}$
- The term symbol of the ground state of sodium is $3^2S_{1/2}$ and that of its first excited state is $3^2P_{1/2}$. The possible quantum numbers n, l, j, and mj of the outer electron in each case is:
  - $3^2S1/2$: n = 3, l = 0, j = ½, m_j = +1/2 or – ½
  - $3^2P_{1/2}$: n = 3, l = 1, j =3/2, m_j = ±1/2 or ±3/2; n = 3, l =1, j =1/2, m_j = ±1/2
- Why is the $2^2P_{5/2}$ state not possible to exist?
  - A P state has L = 1 and J = L ±1/2, so J = 5/2 is impossible

X-ray Spectra

- Arise from these considerations. The Moseley formula then gives the first transitions for electrons knocked by x-rays.
- $$v = \frac{m(Z-1)^2 e^4}{8\epsilon_0^2 h^3}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) = cR(Z-1)^2\left(\frac{1}{1^2} - \frac{1}{2^2}\right)$$
- $$K_\alpha\ x - rays\ v = \frac{3cR(Z-1)^2}{4}$$
- $E\left(K_\alpha\right) = (10.2\ eV)(Z-1)^2$ helps to estimate the K-alpha line emission in terms of the atomic number Z.
- So for example, cobalt with Z = 27 has a 0.180 nm = 1.8 * 10^{-10} m emission or 1.67 * 10^{18} Hz.