# Atoms and Nuclei PA 322

# Revision Lecture (overview of key concepts/topics)

http://www.star.le.ac.uk/~nrt3/322

# Atomic

## Helium LS-coupling (Non-equivalent electrons) LS-coupling (Equivalent electrons) Hund's Rules j-j coupling Zeeman effect Paschen-Bach effect Hyperfine structure X-ray lines

# **Terminology: Quantum Numbers**

Quantum no.	Name	Allowed values	Amplitudes
n	principal	any +ve integer: 1 … ∞	
-	orbital angular momentum	l=0, 1,n-1	$\left \mathbf{l}\right  = \sqrt{l(l+1)}\hbar$
S	spin	s=1/2	$ \mathbf{s}  = \sqrt{s(s+1)}\hbar$
m	orbital magnetic	m <sub>l</sub> = -l, … +l (integer steps)	$l_z = m_l \hbar$
m <sub>s</sub>	spin magnetic	$m_s = \pm s$ = $\pm 1/2$	$s_z = m_s \hbar$
j	total angular momentum	j = $   - s  \dots (  + s)$ (integer steps) j = $  \pm 1/2$ for single electron	$\left \mathbf{j}\right  = \sqrt{j(j+1)}\hbar$
m <sub>j</sub>	total angular momentum projection	m <sub>j</sub> = -j, … +j (integer steps)	$j_z = m_j \hbar$

# Terminology: notation for subshells

The configuration of the *N* equivalent electrons in a given sub-shell is written as

where

• n is principal quantum number (a positive integer)

*I* specifies orbital angular momentum quantum number (allowed values I = 0, 1, ..., n -1)

value of I	0	1	2	3	4	5	6	7	8
letter code /	S	р	d	f	g	h	i	k	

# Terminology: notation for *terms*

Specific configuration of (usually multiple) optically active electron(s), the *spectroscopic term symbol*, is written as:



where

- S is spin quantum number & (2S+1) is spin multiplicity (=2 for a single electron  $\Rightarrow$  called 'doublet')
- *L* specifies overall orbital angular momentum quantum number (in upper case)
- J is total angular momentum quantum number: J = |L-S| ... (L+S)

# **Multiple electron atoms**

- Filled shells can be largely ignored and we are left to deal with the optically active electrons in the outer shell(s).
- If there is only one outer electron, then behaviour is very analogous to H.
- Energy state for electrons in helium:

$$E = E(n,l) + E_{so} + E_{opt.el.}$$
  
binding to spin-orbit coupling interactions (Schr. eqn.)

# Total spin angular momentum

- *Total* spin angular momentum in helium
  - two electrons in ground state must have m\_s= +½ and m\_s=- ½ (PEP)



- excited states (e.g. 1s2s ...) can have spins parallel or anti-parallel
  - parallel spins: triplet states (S=1)
  - anti-parallel spins: singlet states (S=0)
  - states have different energies
    - triplet has lower energy



# **Transitions in helium**

- Consider transitions involving just one electron
- Selection rules forbid transitions between singlet and triplet states
- Hence:
  - absorption lines are all between singlet states
  - emission lines (e.g. from discharge tube which populates various excited states): two distinct sets of lines corresponding to
    - singlet  $\leftrightarrow$  singlet states
    - triplet  $\leftrightarrow$  triplet states

# Spin-orbit coupling for helium (L-S coupling)

- Spin-orbit coupling in helium involves coupling of *total* spin angular momentum with *total* spin angular momentum, ie. J = L + S
  - for singlet states with S=0 no spin-orbit coupling (J = L)
- For triplet states (S = 1) possible values of quantum number J are

J = L+1, L, L-1

and each J state is (2J+1)-fold degenerate according to value of m<sub>J</sub>



# Spectra of general many-electron atoms

- Un-paired electrons are "optically active"
- We considered two schemes:
  - L-S (= Russell-Saunders) coupling, valid for low-Z species
    - terms for *non-equivalent* electrons
    - terms of *equivalent* electrons (same n,l)
    - Hund's rules for L-S coupling: predict the ground state configuration
  - j-j coupling, valid for high-Z atoms (when spin-orbit coupling dominates)

# Terms for *non-equivalent* electrons in many-electron atoms

• i.e. active electrons which belong to different (n,l) sub-shells.



• Example of 2010 paper question 2(b):

What are the possible term symbols for an atom with a 2s 2p electronic configuration, ie. an atom with s and p optically active electrons?

- (e.g. could be an excited state of Beryllium):
- $L = |I_1 I_2| \dots (I_1 + I_2)$  but  $I_1 = 0$   $I_2 = 1 \Rightarrow L = 1$ , so we know the terms must all be P

- S =  $|s_1 s_2| \dots (s_1 + s_2) \Rightarrow$  S =0, 1 since  $s_1 = s_2 = \frac{1}{2}$
- Hence only possibilities are:
  - <sup>1</sup>P, <sup>3</sup>P

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- Finally, consider total  $J = |L-S| \dots (L+S)$ 
  - for <sup>1</sup>P case, L=1, S=0  $\Rightarrow$  J =1; so only term is <sup>1</sup>P<sub>1</sub>
  - for <sup>3</sup>P case, L=1, S=1  $\Rightarrow$  J =0,1,2; so possible terms are  ${}^{3}P_{0,}{}^{3}P_{1,}{}^{3}P_{2}$

# Terms for *equivalent* electrons in many-electron atoms

- More complicated!
- e.g. for 2p<sup>2</sup>:
  - We might expect terms (based on S=0,1 and L=0,1,2):
    - <sup>3</sup>D, <sup>1</sup>D, <sup>3</sup>P, <sup>1</sup>P, <sup>3</sup>S, <sup>1</sup>S
- But <sup>3</sup>D forbidden by Exclusion Principle (both electrons would have same state)
- <sup>3</sup>S and <sup>1</sup>P turn out not to be available due to indistinguishability of electrons.

# Terms for *equivalent* electrons in many-electron atoms

Possible terms for equivalent electrons

ns <sup>0</sup>	<sup>1</sup> S			
ns <sup>1</sup>		<sup>2</sup> S		
ns <sup>2</sup>	<sup>1</sup> S			
np <sup>0</sup>	<sup>1</sup> S			
np <sup>1</sup>		<sup>2</sup> P		
np²	<sup>1</sup> S, <sup>1</sup> D		<sup>3</sup> Р	
np <sup>3</sup>		<sup>2</sup> P, <sup>2</sup> D		<sup>4</sup> S
np <sup>4</sup>	<sup>1</sup> S, <sup>1</sup> D		<sup>3</sup> Р	
np <sup>5</sup>		<sup>2</sup> P		
np <sup>6</sup>	<sup>1</sup> S			

# Hund's rules

Hund's rules tell us which of the allowed terms is ground state:

- 1. state with highest spin multiplicity  $\Rightarrow$   $S_{max}$
- 2. if required, then take term with highest  $L \Rightarrow L_{max}$
- 3. If required:
  - lowest J has lowest energy *if* outermost subshell is less than half full  $\Rightarrow J_{min}$  if q<N/2
  - highest J has lowest energy *if* outermost subshell is more than half full ⇒ J<sub>max</sub> if q>N/2

• For example, 2010 question 2(c):

The possible terms for the ground state of silicon  $(1s^22s^22p^63s^23p^2)$  are  ${}^1S_0$ ,  ${}^3P_{0,1,2}$  and  ${}^1D_2$ . Apply Hund's rules to determine which of these is the ground state term symbol.

- rule 1 selects <sup>3</sup>P<sub>?</sub>
- rule 3 selects <sup>3</sup>P<sub>0</sub> since we are told the outermost subshell is less than half full (3p<sup>2</sup>)

# j-j coupling

- For high Z (and high n at lower Z) the spin-orbit coupling effects for individual electrons become large.
- L-S coupling no longer valid, instead j-j coupling:
  - $\mathbf{j}_1 = \mathbf{l}_1 + \mathbf{s}_1$  for electron 1 -  $\mathbf{j}_2 = \mathbf{l}_2 + \mathbf{s}_2$  for electron 2 ....
  - ... and finally  $\mathbf{J} = \Sigma \mathbf{j}_i$

# Zeeman Effect

When atoms sit in an external magnetic field, energy levels affected by interaction with electron (orbit + spin) magnetic moment.

- Zeeman effect is for case of *weak field*. Produces energy splitting of levels that are otherwise degenerate: m<sub>J</sub> states
  - amplitude of splitting  $\propto |\mathbf{B}|$
  - Normal Zeeman effect:
    - splitting of singlet states (S=0) three lines
  - Anomalous Zeeman effect:
    - splitting of S≠0 states lines ≤ number of transitions

# **Interaction Energy for Zeeman Effect**

Energy depends on magnetic moment

$$\left|\boldsymbol{\mu}_{\mathbf{J}_{\parallel}}\right| = -g\frac{\mu_{B}}{\hbar}\left|\mathbf{J}\right|$$

Where Landé g-factor

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$



# **Interaction Energy for Zeeman Effect**

- Limiting cases:
  - $S=0, L \neq 0 \implies J=L \implies g=1$
  - $S \neq 0, L = 0 \implies J = S \implies g = 2$ 
    - Normal Zeeman means S=0 and thus g=1

– energy difference  $\Delta E_{mag} = \mu_B \Delta m_J$  is same for all L

- -3 distinct components only: corresponding to allowed  $\Delta m_J=0, \pm 1$
- Otherwise "anomalous" Zeeman
  - need to calculate *g* values for particular case.

### Sodium D lines in a weak magnetic field





• Example of 2012 paper question 2(b):

Sketch the weak-field Zeeman energy level diagram for the spectral lines arising from the  ${}^{2}P_{1/2} \rightarrow {}^{2}S_{1/2}$  transition in Sodium, and indicate the quantum numbers of each level.



## **Paschen-Back Effect**



# Hyperfine structure

- Arises due to interaction between nuclear spin angular momentum and the electron total angular momentum.
  - combined spin angular momentum of nucleus called I
    - associated nuclear spin quantum number *I* (0, half-integer or integer)
    - $I_z$  given by projection quantum number  $m_I$  which ranges from -I to +I
  - produces small magnetic moment (typically 1/2000 of electron magnetic moment), hence energies involved small.
  - Combined angular momentum F = I + J (with usual quantisation) leads to line splitting.
  - largest effect for unpaired s-orbital electrons e.g. 21cm line of H



# X-ray spectra

X-rays, being high energy, often involve interactions with low (deep) energy levels in multi-electron atoms.

- Understand the basic features of X-ray spectra as produced by Xray tube:
  - Continuum produced by bremsstrahlung process as electrons are accelerated via interactions with nuclei.
  - Highest energy (smallest wavelength) corresponds to all the electron KE given to producing a single X-ray.



- Overall shape produced by summing up of many cut-off  $I(\lambda) \propto 1/\lambda^2$  spectra.



# X-ray spectra

- Lines arise when electrons drop from higher shells into the "holes" created when a low-lying electron is knocked out of atom.
- Each element exhibits only a few lines, corresponding to transitions between particular low-lying levels (e.g. K $\alpha$  corresponds to n=2 to n=1).
- When plotted against atomic number find  $Z_{eff} \propto \sqrt{\nu}$  (this can be understood due to Coulomb attraction, accounting also for shielding of nuclear charge by any inner electrons).
- Can consider in terms of the transitions of a single hole (similar to transition of a single electron in Alkali metals).





# Nuclear

Scattering theory – cross-sections Mass spectrometer Nuclear force – binding energy Radioactivity - stability Semi-empirical mass formula

# **Nuclear Physics – Basics**

Nucleus of atom is very small (~  $10^{-15}$  m) but has almost all the mass

#### Atomic number Z:

• Z = no.of protons in nucleus

#### Mass number A:

 A = total number of protons (Z) and neutrons (N) in nucleus

#### Notation for specific *nuclide* or *isotope*:



- nuclear masses often quoted in *unified mass unit* designated as "u"
  - u is defined to be 1/12 of mass-energy of an atom of <sup>12</sup>C
  - mass of atom also includes electrons
  - Nucleon masses ~1u
  - 1 u = 931.502 MeV

# **Total cross sections**

Represent the effective "size" of a target particle (atom, nucleus etc.) as seen by an incident particle.

- For scattering in a *thin* foil rate of scattered particles  $R = F_0 \sigma n A \delta x$ (*n* is number density of target foil)
- Scattering by *thick* foil: flux decreases as particles are scattered out of beam  $F = F_0 e^{-n\sigma x}$





# **Differential cross sections**

- Typically interested in angular distribution of scattering  $R(\theta, \phi)$
- For single scattering centre,

$$\frac{R(\theta,\phi)}{F} = \frac{d\sigma}{d\Omega}$$

where  $\frac{d\sigma}{d\Omega}$  is the *differential cross section* 



For thin foil of many scattering centres:  $Rd\Omega = F A n \delta x d\Omega$ 



Integrating gets us back to total cross-section

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega$$

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## Discovery of the nucleus Rutherford scattering

• Scattering rate  $R(\theta)$  into unit solid angle given by *differential cross-section*:



- We see:
  - scattering scales
    - with *nL* = number of scattering atoms per unit area
    - with square of *Z* = charge of nucleus
    - inversely with square of *E* = energy of alphas

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### Nuclear sizes, mass and charge distribution

- Deviation from expected 1/E<sup>2</sup> dependence at large *E* as the alpha particles begin to penetrate nucleus
  - effect sets in at E>25 MeV

- Hence estimate of nuclear size *R* 
  - equate Coulomb potential energy at *R* to particle energy (n.b. alpha particles have charge Ze=2e)

$$E_{\alpha} \approx \frac{2Ze^2}{4\pi\varepsilon_0 R} \implies R = \frac{2Ze^2}{4\pi\varepsilon_0 E_{\alpha}} \approx 10^{-16} Z \,\mathrm{m}$$



• Example of 2012 paper question 3(b):

A beam of  $\alpha$ -particles is incident on an Au foil of thickness 0.5 mm. Using the numbers given below, calculate the fraction of  $\alpha$ -particles which are transmitted through the foil. Number density of Au atoms in the foil  $n = 5.9 \times 10^{28} \text{ m}^{-3}$ Total cross-section for scattering of  $\alpha$ -particles by Au  $\sigma = 1.48 \times 10^{-25} \text{ m}^2$ 

Try thin foil approximation for thickness d=0.0005 m :

Consider a section of foil of area *A*, the total number of Au atoms is *nAd*. Hence fraction of area blocked by Au atoms

fraction scattered =  $nd\sigma$  = 5.9 × 10<sup>28</sup> × 1.48 × 10<sup>-25</sup> × 5 × 10<sup>-4</sup> = 4.3

Hence thin foil approximation is not ok, so try thick film.

fraction transmitted =  $e^{-n\sigma d} = 0.014$ 

## Nuclear sizes, mass and charge distribution

- Electron scattering experiments provide detailed information on nuclear structure
- Implication of electron scattering results:
  - central charge density ≈ constant ⇒ density of nucleons ~ constant and R = R<sub>0</sub> A<sup>1/3</sup>
- Experimentally R<sub>0</sub>=1.23 fm

 $\rho_{nucleus} \sim 10^{12} \text{ x normal matter}$ 



### **Mass spectrometer** Determination of nuclide masses and abundances

Key technology for determination of nuclide masses and abundances. Four components:

- Ion source
- "velocity selector" only allows small range in *v* to pass through. Relies on E and B fields producing forces in opposite directions.
- "momentum selector" uniform magnetic field <u>B<sub>2</sub></u> separates ions by momentum and hence mass (since single value of velocity).
- Detector measures relative positions.



## **Mass spectrometer**



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# **Binding energy**

 Binding energy of a nuclide <sup>A</sup><sub>z</sub>X is difference between its mass energy and that of its constituent nucleons, ie.

$$B = [Z m_p + N m_n - \{m(^{A}X) - Zm_e \}]c^2$$

nucleons mass energy of nuclide = mass of atom minus mass of electrons

# Binding energy per nucleon as function of A





Stable nuclides are shaded black - even-even preferred, odd-odd very rare, due to pairing of nucleons. Line of stability deviates from one-to-one as more neutrons required in heavier nuclei to dilute the Coulomb repulsive force.

Unstable (radioactive) nuclides are shaded grey.

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# **Nuclear force**

Strong nuclear force between nucleons must overcome Coulomb repulsion on short scales:

- Hence attractive and short range.
- Explained by exchange of virtual mesons (and at a deeper level is a consequence of the colour force between quarks).
- Mass of meson ( $m_{\pi} c^2 \approx 100 \text{ MeV}$ ) determines maximum range via Heisenberg UP.



- Complex in detail, so work with approximation schemes.
- Affects protons and neutrons equally, but spin dependent so nucleons "pair up".

# Liquid drop model and the semi-empirical mass formula (SEMF)

- The liquid drop model provides an approximate **formula** for the binding energy *B*(*Z*,*A*) for a nucleus with atomic number *Z* and mass number *A* 
  - Terms in equation motivated by theory, coefficients  $(a_1, \ldots, a_5)$  from experiments.
  - Particularly good when A is large.
  - +ve terms increase binding energy and represent attractive forces etc.

$$B(Z,A) = a_1 A - a_2 A^{\frac{2}{3}} - a_3 Z(Z-1) A^{-\frac{1}{3}} - a_4 \frac{(A-2Z)^2}{A} + \delta(Z,A) a_5 A^{-\frac{3}{4}}$$

Volume / Surface / Coulomb / Symmetry / Pairing

Volume term:



• Explanation: nuclear force has short range, each nucleon only experiences effect of its nearest neighbours ⇒ contribution to binding energy thus scales directly with number of nucleons *A*, so is proportional to volume.

Surface term:



• Explanation: nucleons at the "surface" of the nucleus have fewer neighbours, this term thus effectively corrects the volume term. The surface area of a sphere  $\propto R^2$ , but as we know nuclei have radii  $R \propto A^{1/3}$ , the surface term  $\propto A^{2/3}$ 

Coulomb term:

$$-a_3Z(Z-1)A^{-\frac{1}{3}}$$

- Explanation: the Coulomb term accounts for the electrostatic repulsion between the Z protons in the nucleus. Each proton interacts with (Z-1) other protons (it doesn't interact with itself).
- The potential energy for a sphere of charge *Z* and radius *R* can be shown to be  $\propto Z(Z-1)/R$ , recalling  $R \propto A^{1/3}$

Symmetry term:

$$-a_4 \frac{\left(A - 2Z\right)^2}{A}$$

- Explanation: This term reflects the observed fact that light nuclei have *N*~*Z*. Exactly equal numbers of neutrons and protons gives minimum zero for this term. Factor 1/A means this effect becomes less important as A increases.
- Has origin in the *Pauli Exclusion Principle* applied to nucleons and the way that it effects the filling of nuclear shells in the shell structure of the nucleus.

Pairing term:



- $\delta = +1 Z, N \text{ even}$   $\delta = 0 A \text{ odd}$  $\delta = -1 Z, N \text{ odd}$
- Explanation: term reflects pattern of *Z*, *N* values found in stable nuclei: even-even combination strongly preferred, followed by even-odd or odd-even combinations and very few odd-odd cases. Encapsulates spin-coupling effects in the nucleus. The factor  $A^{-\frac{3}{4}}$  is empirically determined
- Term is +ve for even-even combinations (i.e. increased binding energy).

# Application of the Semi-empirical mass formula

 Values of coefficients (would be given if required in exam) a<sub>1</sub>=15.3 MeV a<sub>2</sub>=16.8 MeV a<sub>3</sub>=0.72 MeV a<sub>4</sub>=24 MeV a<sub>5</sub>=34 MeV

- Semi-empirical mass formula can be used to predict via binding energies
  - stability of isotopes
  - energy changes in nuclear processes and reactions