

PHY2005

Atomic Physics

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(8) Multi-electron atoms: Hartree Theory (and results/screening)

Learning goals

1. To introduce the central field approximation
2. To understand how the central field approximation is used in *Hartree* theory to approximately determine the wavefunctions of multi-electron atoms
3. To outline the concepts of the electron shell / sub-shell structure of atoms
4. To introduce the concepts of effective nuclear charge and electron screening
5. To understand how the effective nuclear charge can be used to estimate the energies of electrons in multi-electron atoms
6. To understand how the screening of electrons relates to their principle (n) and orbital angular momentum (l) quantum numbers
7. To appreciate how the *Aufbau* principle can be used to determine the ground state configurations of atoms

Central field approximation

The Hamiltonian for multi-electron atom:

$$\hat{H} = \sum_i \left[-\frac{\hbar^2}{2m_e} \nabla_i^2 - \frac{Ze^2}{4\pi\epsilon_0 r_i} + \sum_{i>j} \frac{e^2}{4\pi\epsilon_0 r_{ij}} \right]$$

Approximate it with

$$\hat{H} = \sum_i \left[-\frac{\hbar^2}{2m_e} \nabla_i^2 + U(r_i) \right]$$

The potential $U(r_i)$ is chosen to include the **attractive potential** of the nucleus and the **average radial effect of the electron repulsion** felt by one electron as a consequence of all others.

Known as a **central field approximation**.

Hartree method

How do we find $U(r_i)$?

In the **Hartree method** this is done by iteration:

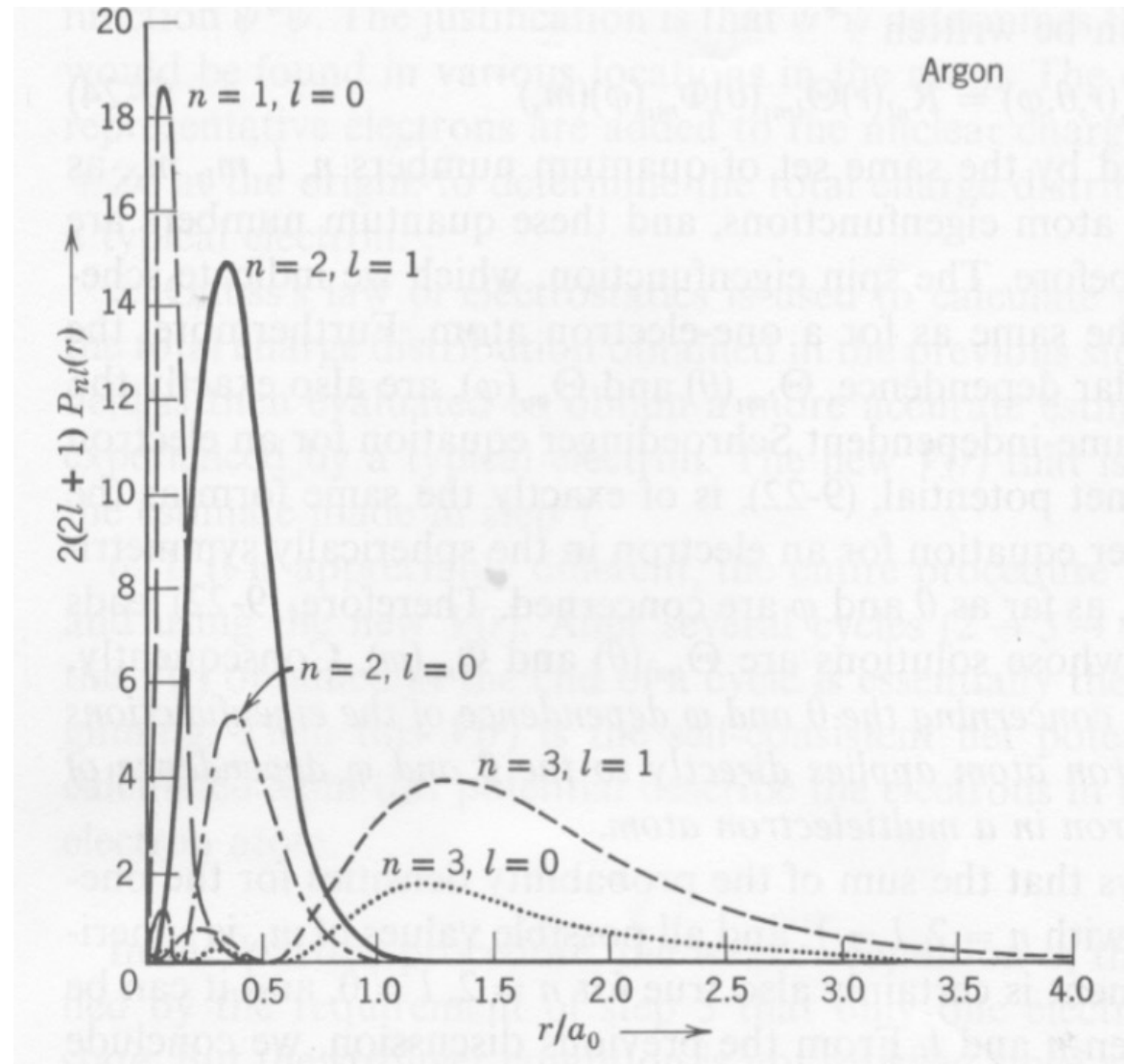
1. Start with a guess
2. Solve for the orbitals
3. Calculate the charge density from the resulting wavefunction
4. Find average spherical charge distribution and then potential from Gauss's Law
5. Repeat steps 2—4 until self-consistent

Provides a new set of orbitals (still n, l, m , quantum numbers) that more accurately reflect the internal structure than purely hydrogenic orbitals.

Hartree method: example

Argon atom (ground configuration): from Eisberg & Resnick:

- Clear shell structure
- Innermost shell smaller than $n=1$ in hydrogen
- Outermost shell comparable to hydrogen

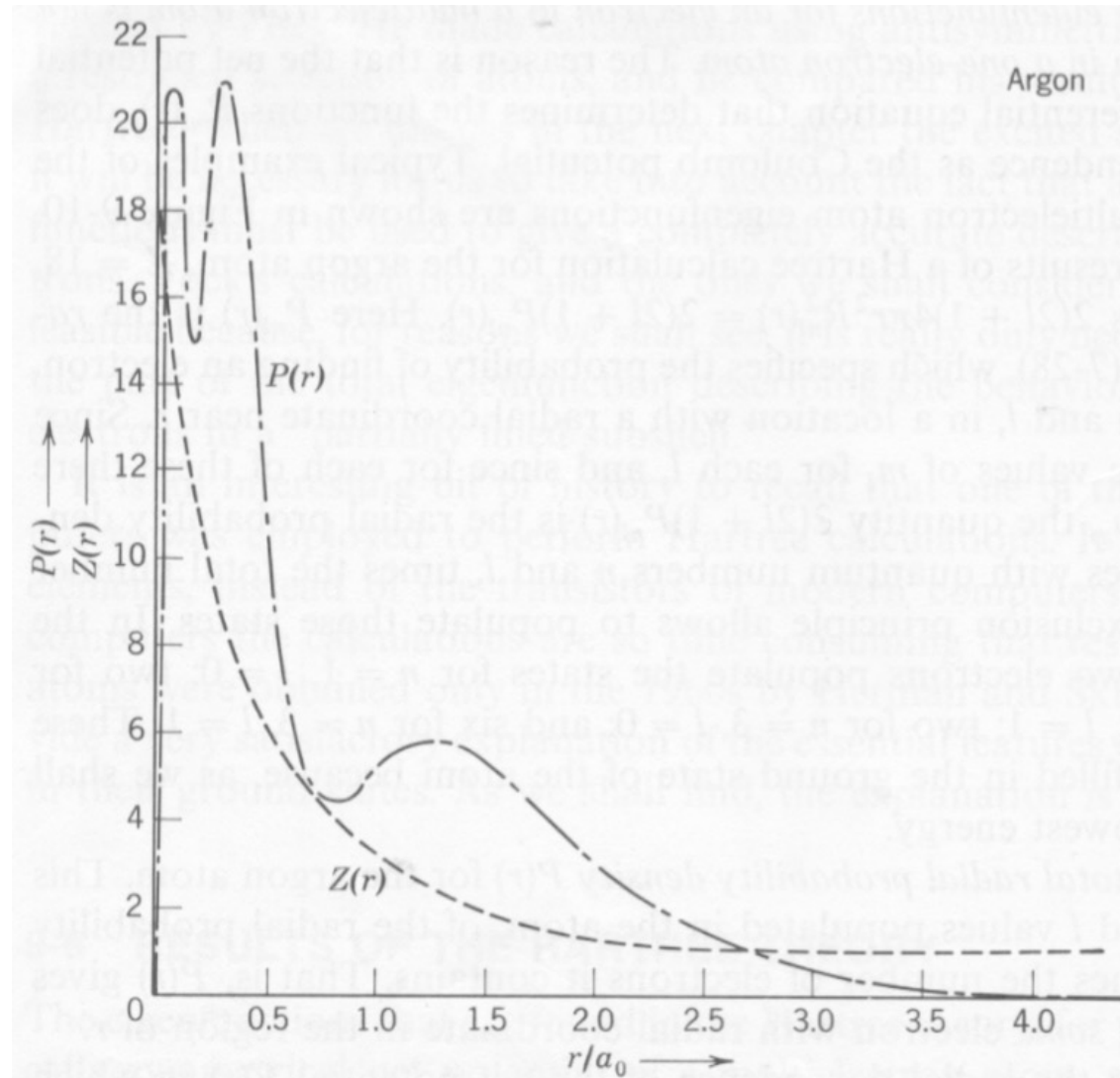


Hartree method: example

Argon atom (ground configuration): from Eisberg & Resnick:

- Potential described by an effective (nuclear) charge, $Z(r)$
- Has anticipated form
- For each shell, can identify an (approximate) value Z_n to use: i.e. as if electrons in that shell move in potential

$$V(r) = -\frac{Z_n e^2}{4\pi\epsilon_0 r}$$



Hartree method: effective charge

Can use effective charge to estimate electron energies:

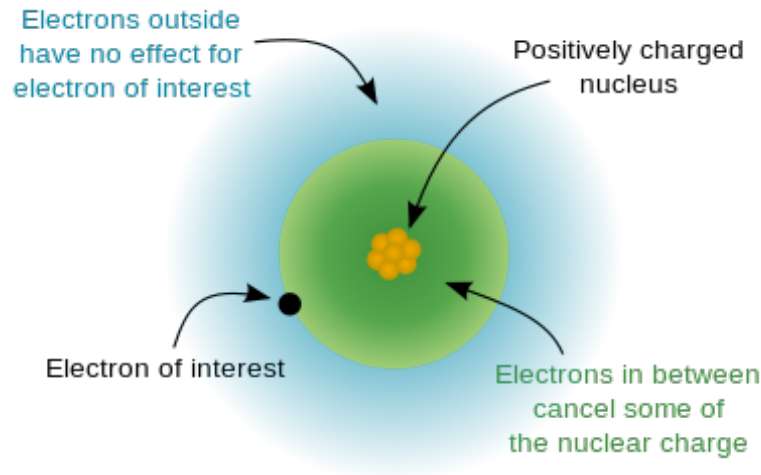
$$E_n \approx -\frac{\mu Z_n^2 e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2} \approx -13.6 \text{ eV} \frac{Z_n^2}{n^2}$$

Important (general) conclusions from Hartree calculations for atoms:

1. For $n=1$, typically find $Z_1 \sim Z - 2$.
 - $n=1$ **shell smaller** than in hydrogen
 - $n=1$ **energy larger** than in hydrogen (see formula above)
2. For outermost shell, typically find $Z_n \approx n$ (very rough)
 - atomic radius grows **very slowly** with atomic number
 - energies of outer electrons **comparable to hydrogen**

Electron screening

Variation in effective nuclear charge can be understood in terms of screening of nucleus by inner electrons:



Recall: **Gauss's Law of electrostatics** tells us that, if spherical, the potential depends only on total charge enclosed.

Thus inner shell electrons can effectively “cancel out” part of the nuclear charge as seen by outer electrons.

Electron screening

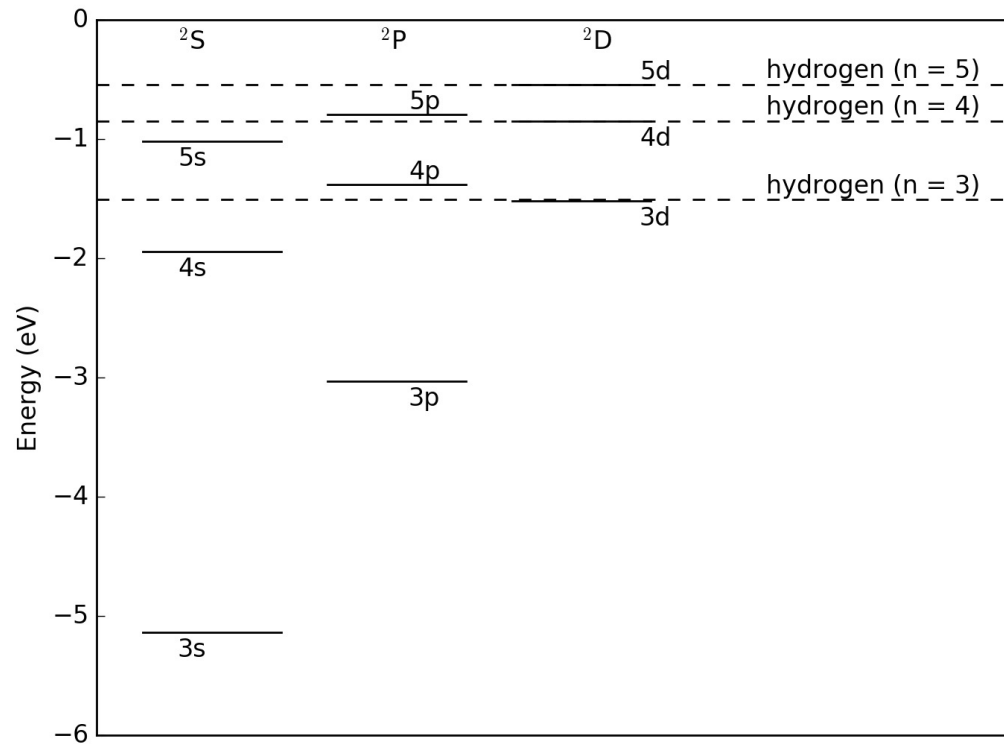
Screening is imperfect: electrons not really localized

Effectiveness of screening depends on orbital angular momentum quantum numbers.

In particular, $l = 0$ orbitals (i.e. s electrons) are better at screening, and harder to screen, since their probability distributions are larger near the nucleus compared to higher l states.

Electron screening in Alkali atom

Screening considerations explain energy levels of alkali atoms such as sodium(shown):



Energy of outer electron is much lower than in hydrogen for s states (relatively poor screening) but gets closer and close to hydrogen for higher l values.

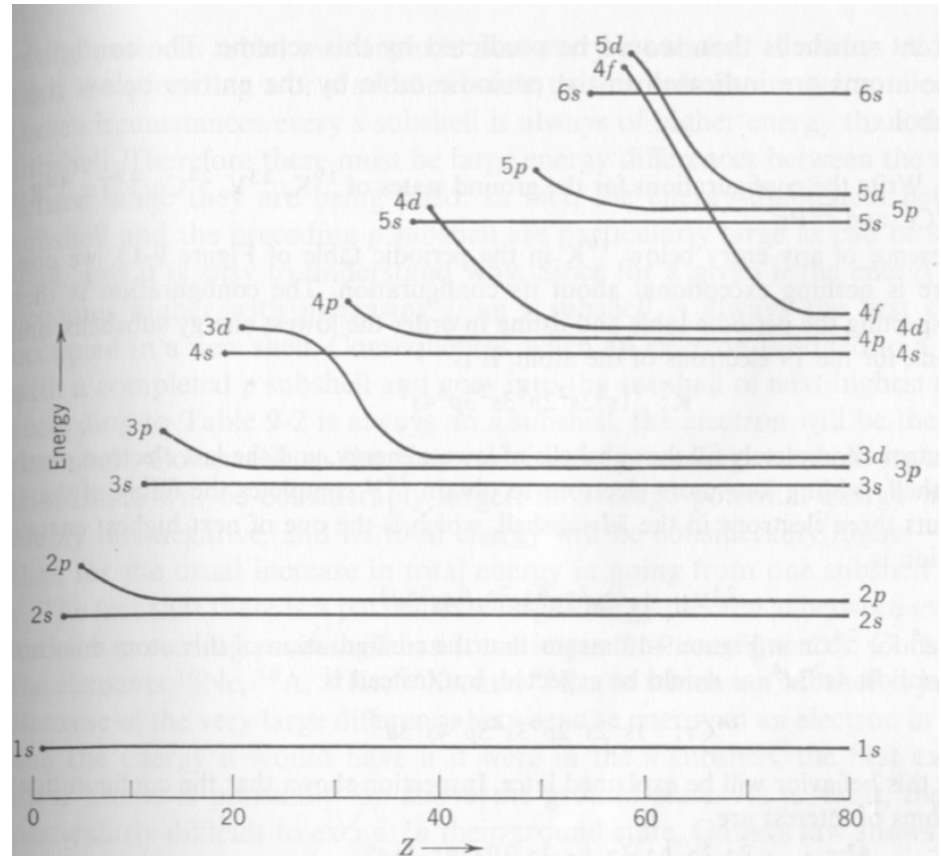
Ground states of atoms:

Aufbau principle

Variations in screening in multi-electron atoms means that the energy ordering of the orbitals varies:
(figure from Eisberg & Resnick)

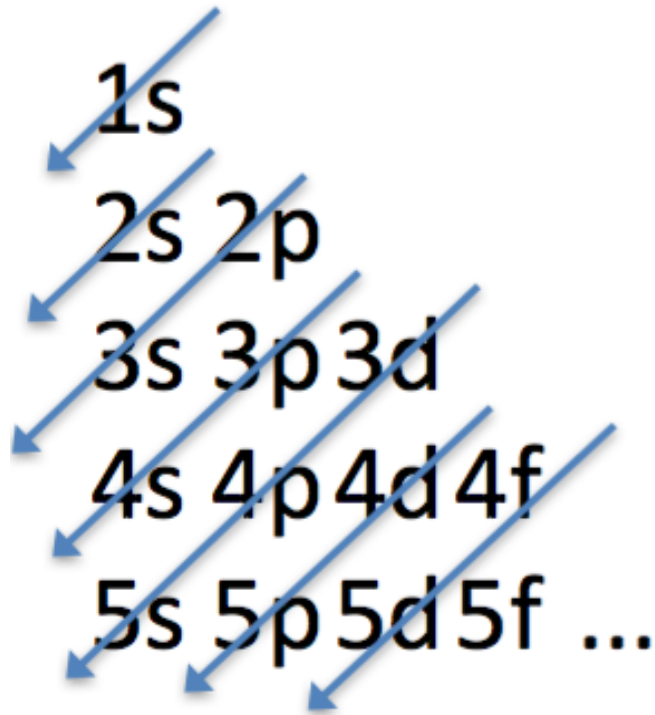
Aufbau principle states that orbitals fill from lowest energy upwards:

- Used to **find the ground configuration** for multi-electron systems



Ground states of atoms: Aufbau principle

Aufbau principle mnemonic:



...usually works, but a few exceptions (e.g. Cr and Cu).

Ground states of atoms: Aufbau principle

Aufbau principle and energy ordering of sub-shells is key to understanding chemical properties and the period table:

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2
IIA
2A

13
IIIA
3A

14
IVA
4A

15
VA
5A

16
VIA
6A

17
VIIA
7A

18
VIIIA
8A

1
H
Hydrogen
1.008

3
Li
Lithium
6.941

4
Be
Beryllium
9.012

11
Na
Sodium
22.990

12
Mg
Magnesium
24.305

19
K
Potassium
39.098

20
Ca
Calcium
40.078

37
Rb
Rubidium
84.468

55
Cs
Cesium
132.905

87
Fr
Francium
223.020

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Helium
4.003

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Ne
Neon
20.180

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39.948

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Summary revision:

- The *central field approximation* to the potential energy allows us to capture many of the important effects of the electron-electron repulsion terms in multi-electron atoms.
- In the central field approximation we include a radial charge distribution in the calculation of the potential energy to account for the average properties of the electrons in the atom.
- In *Hartree Theory* the central potential is determined self-consistently by iteration and electron orbital wavefunctions can then be calculated.
- *Hartree Theory* explains the approximate localisation of electrons in shells and sub-shells with the atom and can roughly be described in terms of effective values for the potential energy in the region of each shell.
- Electrons in multi-electron atoms are *screened* from the full nuclear charge by the net charge distribution of all the other electrons. Inner shell electrons are most effective at shielding outer shell electrons, although the extended charge distributions mean that screening is imperfect.
- Screening of electrons with low l quantum numbers (particularly $l = 0$) is relatively ineffective compared to screening of high- l electrons with the same value of n .
- The configurations of the ground states of atoms can be determined from the *Aufbau* principle: the available sub-shells in that atom are filled systematically, starting with the lowest energy.
- The energy ordering of sub-shells varies from one atom to the next owing to difference in the effectiveness of screening for atoms with differing numbers of electrons.