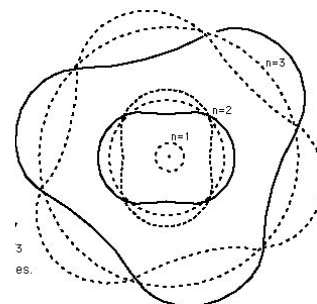


## The Quantum Mechanical (Wave-Mechanical) Model of the Atom

As we have seen, light has both wave-like and particle-like properties. Although Bohr's equations worked for hydrogen, he could not explain why these energy levels existed. In addition, Bohr could not explain the behaviour of atoms with more than 1 electron accurately.

### Louis de Broglie (1923)

- De Broglie considered the wave-particle duality of light and applied it to matter.
- He proposed that electrons exist as “matter waves”. Experiments later proved his theory correct.
- All matter has both wave and particle properties, but the wave-like properties are more significant for objects of very low mass such as electrons.



### Erwin Schrodinger (1925)

- Using de Broglie's idea of an electron wave, he proposed that electrons could only exist in stable waves around the nucleus.
- Since the wavelength of an electron must be a whole number, only certain quantized energies are allowed.
- Schrodinger developed the wave-mechanical equation:

$$\left( \frac{\partial^2 \Psi}{\partial x^2} \right) + \frac{8\pi^2 m}{h^2} (E - V) \Psi(x) = 0$$

$\partial$  = derivative

$\Psi$  = wave function

$x$  = position in 1 dimension

$h$  = Planck's constant

$E$  = total energy

$V$  = potential energy

- This equation describes the energy and motion of an electron around the hydrogen atom in 1 dimension ( $x$ ).
- Schrodinger's equation can be solved to obtain wave functions ( $\Psi$ ) which describe the location in space ( $x, y, z$ ) where an electron is likely to be found.
- These regions are known as **orbitals**.

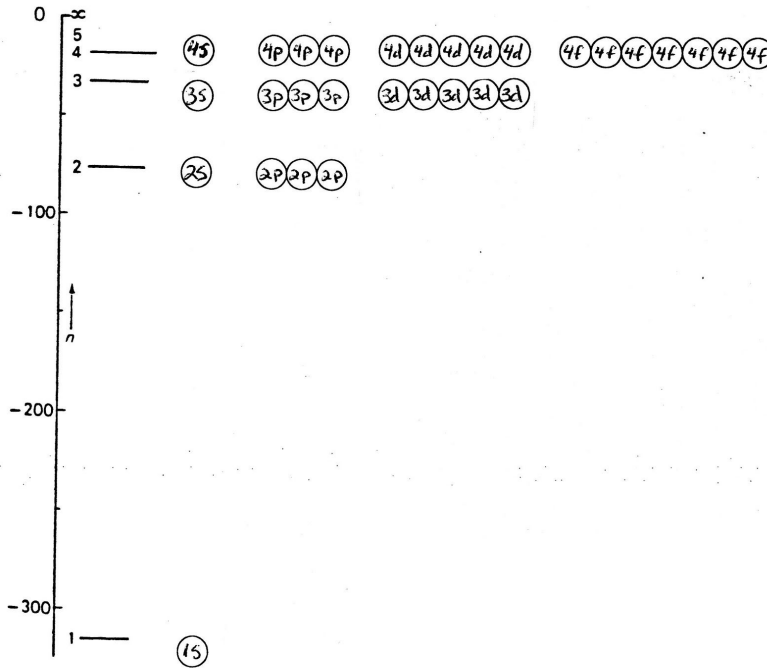
### Werner Heisenberg and The Uncertainty Principle (1927)

- Proposed that it is impossible to determine simultaneously the exact position and velocity (energy) of a single subatomic particle.
- Schrodinger's wave functions actually describe probability distributions or orbitals for where an electron *may* be found.
- Therefore, it is impossible to know everything about a system at the quantum scale; this is not a failure of our ability to measure a system precisely enough (the classical view) but rather is a

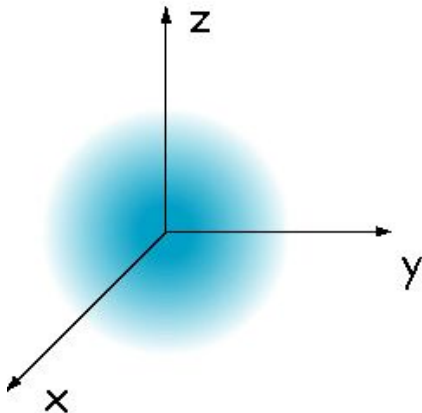
property of microscopic particles such as electrons and protons.

## Orbitals

- At each energy level,  $n$ , there is a probability distribution for where an electron may be found. These are known as orbitals.
- Orbitals have various shapes denoted by the letters s (1 type), p (3 types), d (5 types) and f (7 types).
- The first 3 energy levels of hydrogen contain the following orbitals:

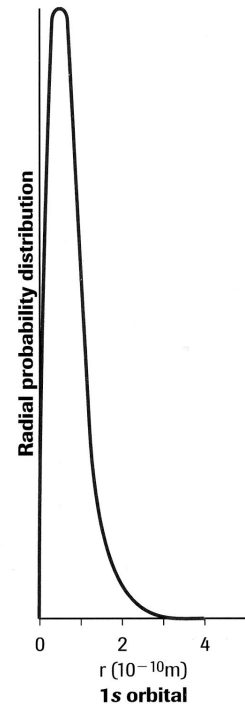


For hydrogen, the ground level state is  $n=1$  or the first ( $1s$ ) orbital. The distance of an electron from the nucleus can only be predicted as a radial probability distribution. In 3 dimensions, the  $1s$  orbital can be imagined as a spherical “cloud” of electrons around the nucleus.

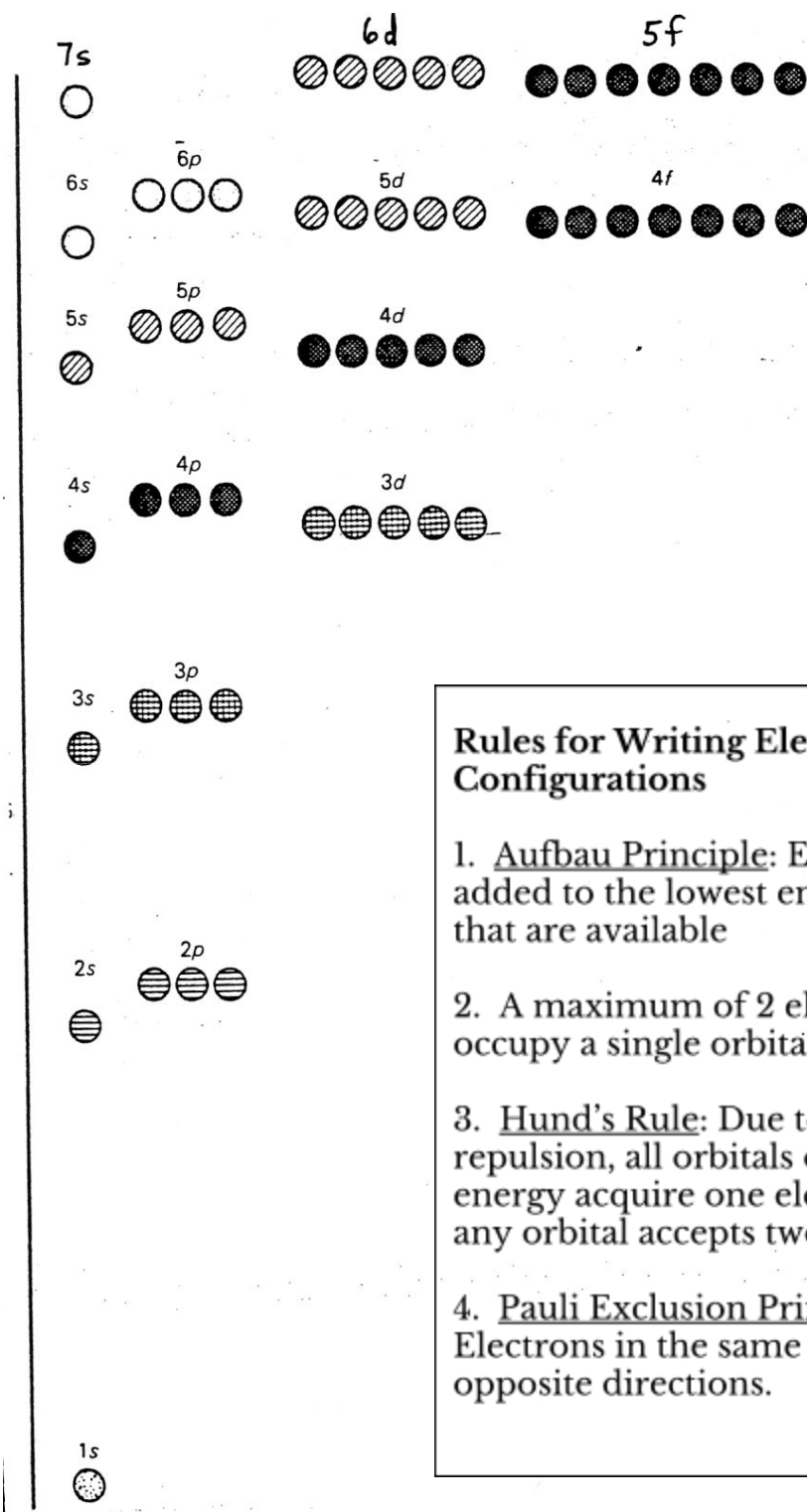


## Multi-Electron Atoms and Ions

With atoms and ions with more than 1 electron, factors such as inter-electron repulsion cause the energy level diagram to be modified.



This energy level diagram shows relative energies of the various orbitals and can be used for dealing with all atoms of the periodic table.



**Rules for Writing Electron Configurations**

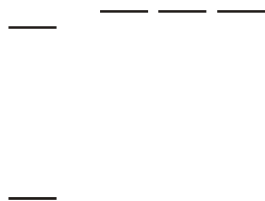
1. Aufbau Principle: Electrons are added to the lowest energy orbitals that are available
2. A maximum of 2 electrons can occupy a single orbital.
3. Hund's Rule: Due to electron repulsion, all orbitals of equal energy acquire one electron before any orbital accepts two electrons.
4. Pauli Exclusion Principle: Electrons in the same orbital spin in opposite directions.

# Energy Level Diagrams

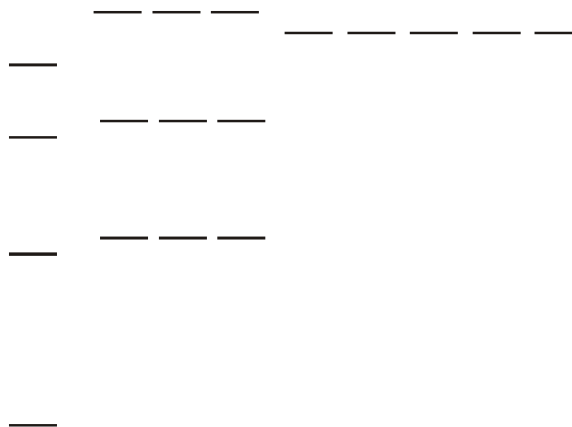
This is a useful tool to visualize orbitals and their relative energies. Electrons are added to an energy level diagram using the same rules describe for writing electron configurations.

Examples:

a) Carbon

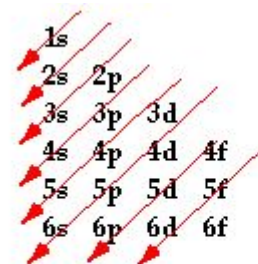


b) Chromium\*



\* Note that the actual electron configuration of chromium is anomalous.

An aufbau diagram (right) is one way to memorize the order in which energy levels are filled. The diagonal arrows indicate the order in which electrons are added to the various orbitals.



# Electron Configuration and the Periodic Table

Sublevels <i>s</i> -block being filled												<i>p</i> -block					
		<i>d</i> -block															
1s	1 2 H He											5 6 7 8 9 10 2p B C N O F Ne					
2s	3 4 Li Be											13 14 15 16 17 18 3p Al Si P S Cl Ar					
3s	11 12 Na Mg	3 4 5 6 7 8 9 10 11 12 3d 21 22 23 24 25 26 27 28 29 30 Sc Ti V Cr Mn Fe Co Ni Cu Zn							31 32 33 34 35 36 4p Ga Ge As Se Br Kr								
4s	19 20 K Ca	39 40 41 42 43 44 45 46 47 48 4d Y Zr Nb Mo Tc Ru Rh Pd Ag Cd							49 50 51 52 53 54 5p In Sn Sb Te I Xe								
5s	37 38 Rb Sr	71 72 73 74 75 76 77 78 79 80 5d Lu Hf Ta W Re Os Ir Pt Au Hg							81 82 83 84 85 86 6p Tl Pb Bi Po At Rn								
6s	55 56 Cs Ba	103 104 105 106 107 108 109 6d Lr															
7s	87 88 Fr Ra																
		<i>f</i> -block															
4f	Lanthe series	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	Actinide series	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 Md	102 No		

## Sample Problems:

1. Write the ground state electron configurations for the following atoms:

Full

Shorthand

- a) beryllium
- b) carbon
- c) oxygen
- d) chromium



## Electron Configurations of Ions

**Anions** (negatively-charged ions) can be written simply by adding the number of electrons corresponding to the ionic charge and then drawing the electron configuration.

e.g. fluorine atom has 9 electrons, therefore the fluoride ion ( $F^-$ ) has 10

fluorine atom (F)

fluoride ion ( $F^-$ ):

**Cations** (positively-charged ions) can be written by first drawing the neutral atom and then removing electrons. *Always remove electrons from the orbitals with the highest principle quantum number first!*

e.g. sodium atom (Na)

sodium ion ( $Na^+$ )

Note that the fluoride ion, neon atom and sodium ion are all isoelectronic (i.e. they have the same electron configurations).

**Transition Metals:** Bohr's model could not explain the charges of the transition metals.

The stable ions of iron can finally be explained by looking at their energy level diagrams. Electrons are always removed from the orbital with the highest principle quantum number first.

e.g. iron atom (Fe):

iron ion ( $Fe^{2+}$ ):

iron ion ( $Fe^{3+}$ ):

### Practice:

Complete Q. 1 – 9 of the worksheet “SP02: The Quantum Mechanical Model of the Atom”, and Q. 1, 2, 7-9 of the worksheet “SP03: Quantum Numbers and Energy Level Diagrams.”



