Quantum Mechanics

Wave Properties of the Electron
Chapters 7-8

De Broglie Wavelength

- Light exhibits some of the same properties as matter, as demonstrated by the photoelectric effect.
- Louis Victor de Broglie hypothesized that matter might exhibit some of the same properties as energy (waves). He derived the de Broglie wavelength for moving particles.
- Consider the equation relating Energy and wavelength:

$$\lambda = \frac{hc}{E}$$

De Broglie Wavelength (continued)

- If energy is substituted with the E of Einstein's equation, **$E=mc^2$**, the equation becomes:

$$\lambda = \frac{hc}{E} \rightarrow \lambda = \frac{hc}{mc^2}$$

- The particle is traveling at some velocity (**v**) slower than the speed of light. Therefore **c** is replaced with **v**, and the equation becomes the De Broglie wavelength: $\lambda = \frac{h}{mv}$

De Broglie Wavelength (continued)

- The wavelength is only of significance if the particle in question is VERY small.
- *Example 1:* What is the wavelength of an electron traveling at 80% of the speed of light?
  $m_e = 9.11 \times 10^{-31}$ kg

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}\ \text{J}}{9.11 \times 10^{-31}\ \text{kg} \bullet (0.8)(3.00 \times 10^{8}\ \text{m/s})}$$

$$\lambda = 3.0 \times 10^{-12}\ \text{m} = 3.0\ \text{pm}$$

Radius of H atom ≈ 3.7×10^{-11} m or 37pm; therefore, the electron has a wavelength on the same scale as the size of the atom.

De Broglie Wavelength (continued)

- *Example 2 :* What is the wavelength of a jogger with a mass of 72 kg traveling at 2.2 m/s?

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}\ \text{J}}{72\ \text{kg} \bullet 2.2\ \text{m/s}}$$

$$\lambda = 4.2 \times 10^{-34}\ \text{m}$$

Height of jogger ≈ 1.8 m. Therefore, the wavelength of the jogger is negligible relative to the overall size of the jogger.

Development of the Quantum Mechanical Model of the Atom

- In Bohr's model, we considered the electrons orbiting the nucleus like planets around a sun.
- If this model were correct, the electrons should spiral into the nucleus.
- Generally speaking, electrons do not collide with the nucleus – the planetary model is NOT correct.
- However, the concept of Bohr's ENERGY LEVEL (n) does hold up to experimentation and is the basis of the quantum mechanical model of the atom.

Quantum Mechanical Model of the Atom (continued)

- The Heisenberg uncertainty principle says that there is a limitation to how precisely we can know the speed and position of a moving body:

$$\Delta x \bullet \Delta(mv) \geq \frac{h}{4\pi}$$

- This uncertainty is only significant for small, fast-moving particles, like an electron.

Quantum Mechanical Model of the Atom (continued)

- The quantum (or wave) mechanical model was proposed by Erwin Schrödinger.
- He treated the electron mathematically as a wave function, describing its position in space as a function of its x,y, and z coordinates:

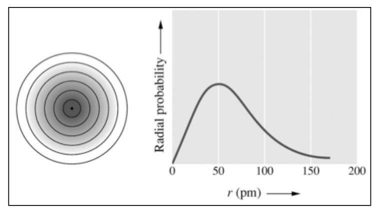
$$H(\Psi) = E\Psi$$

where H is a mathematical operator, E is energy, and Ψ is a wave function (a treatment of the electron as a standing wave).

The standing waves caused by the vibration of a guitar string fastened at both ends. Each dot represents a node (a point of zero displacement).

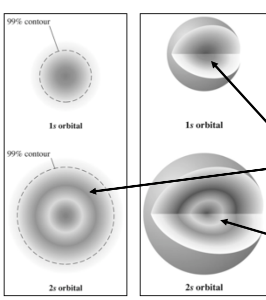
The hydrogen electron visualized as a standing wave around the nucleus. Notice that only whole numbers will work.

Quantum Mechanical Model of the Atom (continued)



- By this treatment, the electron is not considered to "orbit" the nucleus, but instead, it occupies distinct energy levels within an atom.
- Solving the wave function will give an electron probability map, indicating where the electron can be found in the atom a certain percentage of the time.
- The electron moves *randomly* within its electron probability distribution.

Cross-sectional & cut-away representations of the probability distributions of *s* orbitals.



- An electron has a 99% probability of being within the 99% contour line.
- 1% of the time the electron will be outside this region.
- The position and speed of the electron in this space cannot both be known with certainty.

Purple areas represent highest probability of finding an electron.

White circle represents a node.

Quantum Numbers

- A set of ***four*** quantum numbers can be used to describe the energy of and the space where an electron may be found within an atom.
- Every electron in an atom has a ***unique*** set of 4 quantum numbers.
- Quantum numbers can be used with the Schrödinger Equation to determine the wave function and probability map of a specific electron.

The Principle Quantum Number (n)

- The ENERGY LEVEL of the electron.
- n = 1,2,3,4,5,.....(to infinity)
- Corresponds to the Bohr model energy level.
- Corresponds to the ROW of the periodic table.
- The # of electrons in level $n = 2n^2$
- The higher the energy level, the higher the energy of the electron. However, as **n** *increases* the energy difference between adjacent energy levels *decreases*.

The Angular Momentum Quantum Number (l)

- The ENERGY SUBLEVEL of the electron.
- Also indicates the SHAPE of the orbital (region of space occupied by an electron.
- Every energy level (n) can be broken down into n sublevels.
  - *For example, the third energy level can be broken down into three sublevels).*
- l -values range from *zero* to *n-1*.
  - *For example, in the third energy level, the l quantum number can be equal to 0, 1, or 2).*

Sublevels have the following letter designations. Each sublevel has an orbital shape characteristic to it.

ℓ- value	letter	shape
$\ell = 0$	s	Spherical
$\ell = 1$	p	Peanut (figure 8)
$\ell = 2$	d	Four 4-leaf clovers One dumbbell with a donut
$\ell = 3$	f	Flower

The Magnetic Quantum Number (m_ℓ)

- Determines the **orbital** (specific region of space within a sublevel) that an electron occupies.
- The number of orbitals within an energy level, *n*, equals n^2.
- The number of orbitals within a sublevel, ℓ, is equal to $2\ell+1$
- m_ℓ ranges from $-\ell$ to $+\ell$

  For example, if $\ell=2$, m_ℓ may equal -2, -1, 0, 1, 2
- Each orbital in a sublevel has the same shape, but a different orientation in space.
- An orbital may hold up to 2 electrons.

The Spin Quantum Number (m_s)

- Designates the magnetic properties of the electron: Spin.
- Spin is usually considered up or down.

  Spin up is often designated $m_s = +½$

  Spin down is often designated $m_s = -½$.
- Expression of the Pauli exclusion principle:

  Every electron in an atom has a unique set of quantum numbers.

Quantum number designations

How many *orbitals* can have the following designations. Note that some may not be allowed.

- n=6, l=5
- n=6, l=5, m_l=-3
- n=6
- n=9, l=9
- n=3, l=2, m_l=0, m_s=+½
- 3s
- 5f
- 2d

Quantum number designations

How many *electrons* can have the following designations. Note that some may not be allowed.

- $n=5$, $l=3$
- $n=4$, $l=2$, $m_l=0$
- $n=3$, $l=3$, $m_l=-2$
- $n=6$, $l=1$, $m_l=-1$, $m_s=-½$
- 2p
- $2p_x$

Electron Configurations

- A detailed list of energy levels, sublevels, and orbitals of electrons in the atom.
- The "address" of the electrons.

Electron Orbital–Filling in Atoms

- Aufbau Diagram – a map to determine the location of electrons within an atom – helps to write the electron configuration.
- When filling orbital diagrams, follow these rules:
  - **Aufbau principle** – When filling electron orbitals, lower energy orbitals fill first. All of the orbitals of the same sublevel (degenerate = same energy) are filled before a new sublevel begins filling.
  - *Note: The higher the electron energy level in an atom, the more it overlaps with adjacent energy levels.*

Orbital-filling rules (cont.):

- **Hund's Rule** – Place one electron in each orbital of the same sublevel before pairing electrons.
- **Pauli Exclusion Principle** – An orbital may hold a maximum of two electrons with opposite spins. By convention, we will put the first electron with spin up, and the second with spin down.

- Use the Aufbau diagram to write electron configurations for the following atoms:

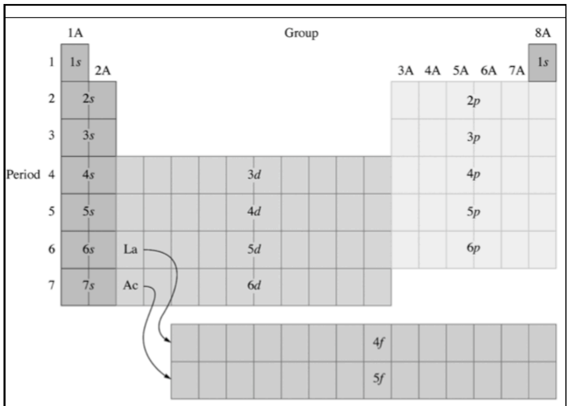
Electron configurations can be written more quickly by looking at the pattern of orbitals and sublevels. The following diagram will help you use these patterns. Simply list the electron orbitals:

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f 5g
6s 6p 6d 6f 6g 6h
7s 7p 7d 7f 7g 7h 7i
8s 8p 8d 8f 8g 8h 8i 8j

Then, use diagonal arrows as below:

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f 5g
6s 6p 6d 6f 6g 6h
7s 7p 7d 7f 7g 7h 7i
8s 8p 8d 8f 8g 8h 8i 8j

Using the diagram above write electron configurations for the following atoms:



Abbreviated electron configurations

- Noble Gases have the most stable electron configurations.
- All noble gases end with an ***octet*** – filled outer s & p energy sublevels (s^2p^6).
- The symbol for a noble gas may be substituted for its electron configuration for writing longer configurations.
- Write abbreviated electron configurations for the following atoms:

Valence & Core electrons

- **Core electrons = inner electrons**
  - In the electron configuration, the core electrons are equivalent to a noble gas configuration (plus any full outer d or f sublevels).
  - These electrons do NOT participate in chemical bonding.
- **Valence electrons**
  - Electrons in the ***outermost s & p*** *sublevels* and ***unfilled d & f*** *sublevels*.
  - These electrons can participate in chemical bonding.

Exceptions to orbital-filling rules

- Transition Metals (d-block)
  - Copper group
  - Chromium group
  - Others:
- Inner transition metals (f-block)
  - $\mathbf{d^1}$ rule and exceptions

Electron Configurations and ION formation

- Many METALS lose electrons to achieve an electron configuration equivalent to a noble gas (an OCTET).
- Many NON-METALS gain electrons to achieve a Noble Gas electron configuration.
- *Transition metals* and *p-block* metals sometimes form ions with a pseudo-Noble Gas electron configuration, or other stable electron configuration.