

Section 3 Notes: The Quantum Theory and Quantum Numbers

Read (p.310-313)

The Bohr Model in which electrons moved in a fixed circular path around the nucleus of an atom could not be made to work. When Bohr's model for calculating the energy of electrons in atoms with more than one electron was applied, his equation just didn't work. **Bohr's equation was fundamentally incorrect.** However, it did show the quantized energy of an electron and paved the way for other theories.

Three physicists, Louis de Broglie, Werner Heisenberg, and Erwin Schrodinger developed new theories based on electrons behaving as **waves**—"wave mechanics" or "**quantum mechanics**". Schrodinger gave emphasis to the wave properties of electrons. Both he and de Broglie said that an electron was bound to the nucleus in a way similar to a *standing wave*. Schrodinger's equation gave us

$$\hat{H}\psi = E\psi$$

Where \hat{H} is a set of mathematical instructions (operation), E is the total energy of the atom, and ψ is the **wave function** of the electron. $E\psi$ came to represent an **orbital**.

The quantum mechanical model of a hydrogen electron in its ground state has a $E\psi$ of **1s**. An "**orbital**" is **not an orbit**. An orbital is a region of space around a nucleus in which an electron with a certain amount of energy most probably moves.

BUT, we do not know how it is moving. If we were to observe its position, we lose its momentum and the wave would collapse. If we observe the momentum, we lose the position.

Heisenberg's mathematical analysis of this problem became known as the **Heisenberg Uncertainty Principle**: *There is a fundamental limit on just how precisely we can know the position and momentum of a particle at a given time.*

Or—It is impossible to know both the position and the momentum of a particle simultaneously.

His equation is $(\Delta X)(\Delta mv) \geq h/4\pi$

X is position

mv is momentum

The minimum uncertainty is $h/4\pi$

This means, the more accurately you know the position, the less accurately you know the momentum and vice versa.

The **square of ψ** does have a definite physical significance. The square of the wave function indicates the **probability** of finding an electron in a particular region of space in the atom. The quantum mechanical model gives the definition of a **1s** orbital in hydrogen as the region around the nucleus that gives a 90% probability of finding an electron.

Quantum Numbers

Read (p. 313-318)

Solving Schrodinger's equation for the hydrogen atom, there are many wave functions (orbitals) that satisfy it. Each orbital is characterized by a series of numbers called **quantum numbers**.

Quantum numbers describe the "properties" of the orbital. There are 4 properties or quantum numbers for each orbital.

First quantum number:

The principal quantum number (n) has integral values: 1, 2, 3.... It is related to the **size** and **energy** of the orbital (energy level). A larger "n" means the electron spends more time further from the nucleus and that the electron is less tightly bound to the nucleus, thereby, having higher energy (less negative).

Second quantum number: Azimuthal Quantum Number:

The angular momentum quantum number (ℓ) has an integral value of (0 to n-1) for each value of "n" and is related to the **shape** of the orbital. Each shape is assigned a letter and each letter has its corresponding number.

For $\ell = 0$ the shape is s s orbitals are spherical

For $\ell = 1$ the shape is p p orbitals are 2-lobed or "dumbbell"

For $\ell = 2$ the shape is d d orbitals are 4-lobed

For $\ell = 3$ the shape is f f orbitals are 8-lobed

(See p.315 to 317 for pictures of the orbital shapes and their orientations.)

(Any orbital, regardless of shape, can hold up to 2 electrons, never more.)

The first energy level, n=1, has only an s orbital because 0 to n-1 would be 0 to 1-1 which is only 0 and 0=s

The 2nd energy level, n=2, has both "s" and "p" orbitals because 0 to n-1 would be 0 to 2-1 or 0 and 1 which is 0=s and 1=p.

The 3rd energy level, n=3, has s, p, and d orbitals because 0 to n-1 would be 0 to 3-1 or 0 to 2 which is 0=s, 1=p and 2=d.

The 4th energy level, n=4, has s, p, d, and f orbitals because 0 to 4-1 is 0 to 3 which is 0=s, 1=p, 2=d, and 3=f.

All energy levels 4 or higher have s, p, d, and f orbitals. **There are also g orbitals but no electron in its ground state is in a g orbital so we will not discuss them.**

Third quantum number:

The magnetic quantum number (m_ℓ) has an integral value ranging from - ℓ to + ℓ including 0. It refers to the orbitals orientation in space relative to other orbitals in the atom.

So if the **shape is s** then its **number is 0** and its **orientation** has to be **0**.

If the **shape is p**, then its **number is 1** and its orientation can be **-1, 0, 1**.

If the **shape is d**, then its **number is 2** and its orientation can be **-2, -1, 0, 1, 2**.

If the **shape is f**, then its **number is 3** and its orientation can be **-3, -2, -1, 0, 1, 2, 3**.

Also note that there can be only be one s-orbital, three p-orbitals, five d-orbitals, and seven f-orbitals on any energy level that contains that shape. (See Table 7.2 on p. 314.)

Shapes and Energies:

s-orbitals have lower energy than p-orbitals which have lower energy than d-orbitals which have lower energy than f-orbitals.

Since electrons will go to lowest energy they fill all the orbitals in a “subshell” (energy level with its shape) before they go to a higher energy level or shape. **Subshells are degenerate, or have the same energy.**

Aufbau Process: There is a **very specific filling order** for orbitals in the electron cloud of atoms.

Hund’s Rule:

Electrons, in an atom, fill orbitals singly before they double, and they fill a subshell before moving to the next.

Although there are a few exceptions to Hund’s Rule, this rule holds true in almost all instances.

Fourth Quantum Number:

Electronic Spin quantum number (m_s) is given the numerical value of $+\frac{1}{2}$ or $-\frac{1}{2}$ and refers to the spin the electron takes on in its orbital. The positive $\frac{1}{2}$ refers to a “clockwise spin” or “up spin”, and the negative $\frac{1}{2}$ refers to a counter-clockwise spin” or “down spin”.

Remember every orbital can hold “up to” two electrons. According to Hund’s Rule, the electrons fill orbitals in a subshell “singly” before doubling. This is because electrons (e^-), having a negative charge, repel other electrons. When they are close to each other in an orbital, they spin in opposite directions reversing their magnetic poles and making it possible to exist in the same region of space. They first fill singly so they can avoid the repulsion.

So the 4th quantum number will be $+\frac{1}{2}$ first until all orbitals are half filled, then $-\frac{1}{2}$ if they need to double up.

***Pauli Exclusion Principle**

No two electrons in the same atom will have the same four quantum numbers.

(s, ℓ, m_ℓ, m_s)

There are not exceptions to the Pauli Exclusion Principle.

Note: A **node** is a region in an orbital where the probability of finding an electron is close to zero.

Please take time to study these section 3 notes. They are a bit tricky and need time to “sink in”.

The last section of this chapter covers Electron Configuration, Orbital Diagrams, and Tendencies in the Periodic Table.

Please watch the second half of Video 5, Electronic Structure of the Atom.

The Aufbau Order will be covered in the next set of notes. I will explain it in detail next section.