

# Quantum Mechanics

Quantum mechanics was initially developed to provide a better explanation of the atom, especially the spectra of light emitted by different atomic species. The quantum theory of the atom was developed as an explanation for the electron's staying in its orbital, which could not be explained by Newton's laws of motion and by Maxwell's laws of classical electromagnetism.

The foundations of quantum mechanics were established during the first half of the twentieth century. Some fundamental aspects of the theory are still actively studied.

Quantum mechanics is essential to understand the behavior of systems at atomic scales and smaller.

For example, if classical mechanics governed the workings of an atom, electrons would rapidly travel towards and collide with the nucleus, making stable atoms impossible. However, in the natural world the electrons normally remain in an uncertain, non-deterministic "smeared" orbital path around or "through" the nucleus, defying classical electromagnetism.

In quantum mechanics, the state of a system at a given time is described by a **complex wave function** (**orbitals** in the case of atomic electrons). This **abstract mathematical region of space** allows for the calculation of probabilities of outcomes of concrete experiments.

## **The Development of Quantum Mechanics**

In 1924, Louis-Victor de Broglie produced a hypothesis, **claiming that all matter, not just light, has a wave-like nature** – or - in terms of electrons, **electrons have wave-like behavior just like photons.**



The de Broglie equations relate the wavelength  $\lambda$  and frequency  $f$  to the momentum  $P$  and energy  $E$ , respectively, as

$$\lambda = \frac{h}{p} \quad \text{and} \quad f = \frac{E}{h}$$

De Broglie's formula was confirmed three years later for electrons (which differ from photons in having a rest mass) with the observation of electron diffraction in two independent experiments.

(G. P. Thomson at the University of Aberdeen, and C.J. Davisson at Bell Labs.)

De Broglie was awarded the Nobel Prize for Physics in 1929 for his hypothesis. Thomson and Davisson shared the Nobel Prize for Physics in 1937 for their experimental work.

## Heisenberg's Uncertainty Principle 1927



In his work on formulating quantum mechanics, Werner Heisenberg postulated his uncertainty principle, which states:

Certain pairs of physical properties, like position and momentum, cannot both be known simultaneously to arbitrary precision. That is, the more precisely one property is known, the less precisely the other can be known. This is not a statement about the limitations of a researcher's ability to measure particular quantities of a system, it is a statement about the nature of the system itself. As a consequence of the uncertainty principle, it is impossible to measure simultaneously both position and velocity of a microscopic particle with any degree of accuracy or certainty.

The uncertainty principle is represented mathematically as:

$$\Delta X \Delta P \geq \frac{\hbar}{2}.$$

In quantum mechanics, a particle is described by a wave. The position is where the wave is concentrated and the momentum is determined by the wavelength. The position is uncertain to the degree that the wave is spread out, and the momentum is uncertain to the degree that the wavelength is ill-defined.

The modern explanation of the uncertainty principle, depends mainly on the wave nature of a particle.

Just as it is nonsensical to discuss the precise location of a wave on a string, particles do not have perfectly precise positions; likewise, just as it is nonsensical to discuss the wavelength of a "pulse" wave traveling down a string, particles do not have perfectly precise momenta (which corresponds to the inverse of wavelength). Moreover, when position is relatively well defined, the wave is pulse-like and has a very ill-defined wavelength (and thus momentum).

And conversely, when momentum (and thus wavelength) is relatively well defined, the wave looks long and sinusoidal, and therefore it has a very ill-defined position.

Werner Heisenberg worked as an assistant to Bohr and university lecturer in Copenhagen from 1926 to 1927. It was there, in 1927, that Heisenberg developed his uncertainty principle, while working on the mathematical foundations of quantum mechanics.

# The Schrödinger Equation 1926



Erwin Rudolf Josef Alexander Schrödinger was an Austrian theoretical physicist who achieved fame for his contributions to quantum mechanics, especially the Schrödinger equation, for which he received the Nobel Prize in 1933.

For a single particle in three dimensions:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}, t) + V(\mathbf{r}) \Psi(\mathbf{r}, t)$$

where:

- $\mathbf{r} = (x, y, z)$  is the particle's position in three-dimensional space,
- $\Psi(\mathbf{r}, t)$  is the wavefunction, which is the amplitude for the particle to have a given position  $\mathbf{r}$  at any given time  $t$ .
- $m$  is the mass of the particle.
- $V(\mathbf{r})$  is the time independent potential energy of the particle at each position  $\mathbf{r}$ .
- $\nabla^2$  is the Laplace operator.

In quantum mechanics, the Schrödinger equation is an equation that describes how the quantum state of a physical system changes in time. It is as central to quantum mechanics as Newton's laws are to classical mechanics.

In the standard interpretation of quantum mechanics, the quantum state, also called a wave function or state vector, is the most complete description that can be given to a physical system. Solutions to Schrödinger's equation describe not only atomic and subatomic systems, atoms and electrons, but also macroscopic systems, possibly even the whole universe.

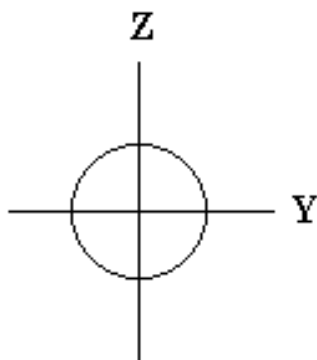
Putting it simply, the equation maps out the 3-D regions of space in which an electron with certain properties is likely to be found. These regions of space are called orbitals. The orbitals each have certain shapes designated as s, p, d and f.

# Atomic Orbitals

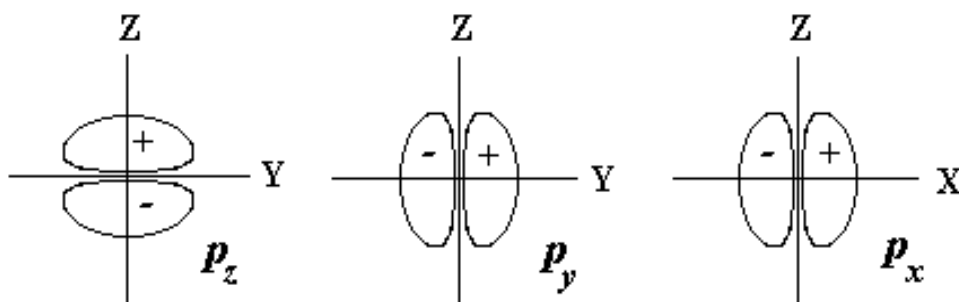
[Link to the Grand Orbital Table in Orbital Viewer](#)

[Link to the Orbitron](#)

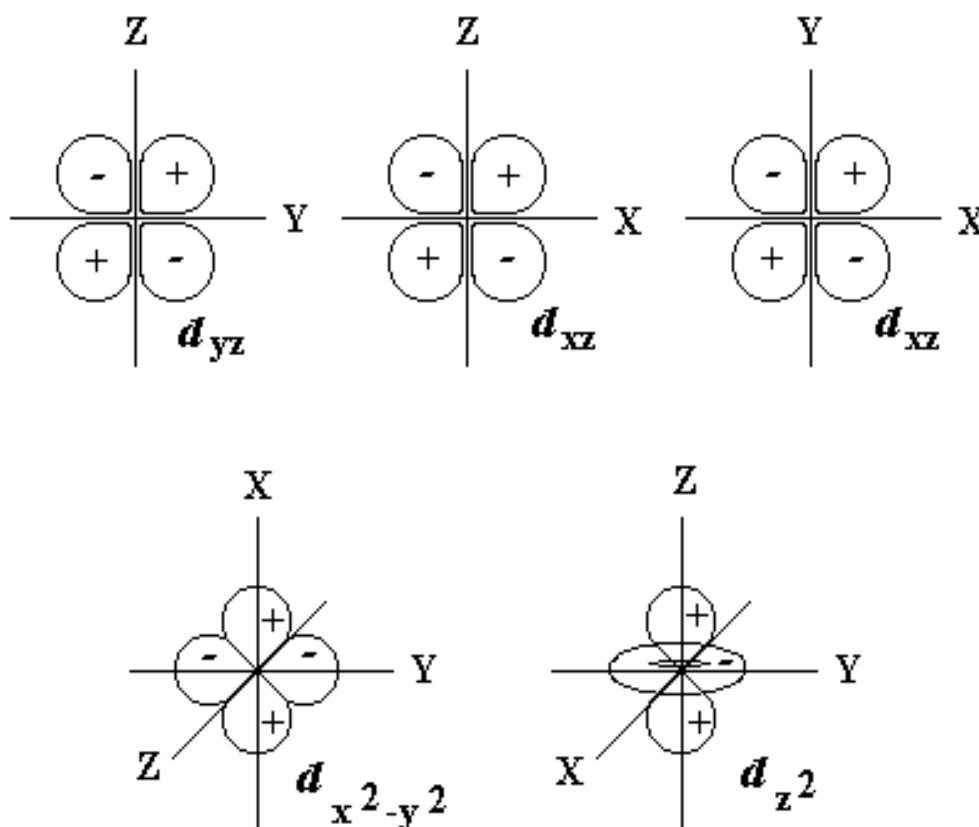
The shapes of orbitals are described by surfaces through regions of equal probability. The shapes most commonly used are those that include 99% probability. An s orbital is spherical and has only one orientation. An s orbital is shown below.



A p orbital is lobe shaped with two parts separated by a nodal plane where the probability is zero. There are three orientations available for a p orbital. They are named  $p_z$ ,  $p_y$  and  $p_x$ . These are shown below.



A  $d$  orbital has four lobes. The probability is zero between the lobes. There are **five possible orientations**. These are shown below.



**Each atomic orbital, regardless of shape, holds a maximum of only 2 electrons.**

We'll omit the  $f$  orbital shapes and beyond from these notes as they are not required information in Mr. Scott's Chemistry I class.

# Quantum Numbers

There are four quantum numbers normally used to describe electrons.

(1) Principle Quantum Number ( $n$ )

$$n = 1, 2, 3, 4 \dots$$

(2) Azimuthal Quantum Number ( $\ell$ ) aka: Orbital Q.N.

$$\ell = 0, 1, 2, 3 \text{ or } (s, p, d, f)$$

(3) Magnetic Quantum Number ( $m_\ell$ )

$m_\ell = x, y, z$  orientation in space

or

(0) for s;

(-1, 0, +1) for p;

(-2, -1, 0, +1, +2) for d; etc...

(4) Spin Quantum Number ( $m_s$ )

$m_s = -\frac{1}{2}$  or counterclockwise

$+\frac{1}{2}$  or clockwise

The next section of notes explains the use of these quantum numbers in establishing electron configuration.